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Pipecolic Acid-Catalyzed Direct Asymmetric Mannich Reactions

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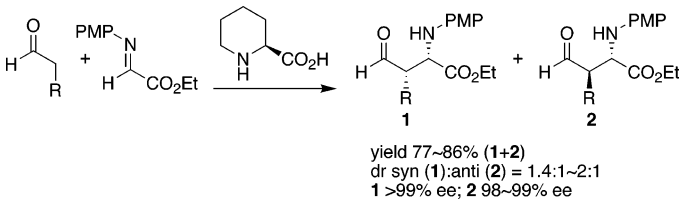
ABSTRACT



Mannich reactions between aldehydes and *N*-*p*-methoxyphenyl-protected α-imino ethyl glyoxylate have been performed using (*S*)-pipecolic acid as catalyst. The reactions give both *syn*- and *anti*-products (dr = 1.4–2:1) with high enantioselectivities (>98% ee). In contrast, (*S*)-proline-catalyzed reactions give mainly *syn*-products with high enantioselectivities. Computational studies reveal that the energetic preference between the transition structures involving the s-*cis*-enamine and the s-*trans*-enamine is smaller for the pipecolic acid as compared to proline, yielding the (2*S*,3*R*)-*anti* and the (2*S*,3*S*)-*syn* Mannich product in nearly equal amounts.

Preformed enamines of both five-membered pyrrolidine and six-membered piperidine rings have been used as nucleophiles in many reactions.[1,2] For the reactions involving in situ-generated enamines, pyrrolidine-based catalysts have been extensively examined.[3−5] One of the most effective routes for the synthesis of enantiomerically enriched α- and β-amino acid derivatives is pyrrolidine derivative-catalyzed Mannich-type reactions of an aldehyde donor. (*S*)-Proline and various (*S*)-proline derivatives give the *syn*-product (2*S*,3*S*)-**1** as the major product with high diastereo- and enantioselectivity (Scheme 1).[4] The six-membered analogue, pipecolic acid, has received little attention as a catalyst for asymmetric reactions and has proven to be ineffective for aldol reactions involving acetone as donor.[3a,6] Here we report the experimental and computational investigation of (*S*)-pipecolic acid-catalyzed Mannich reaction between aldehydes

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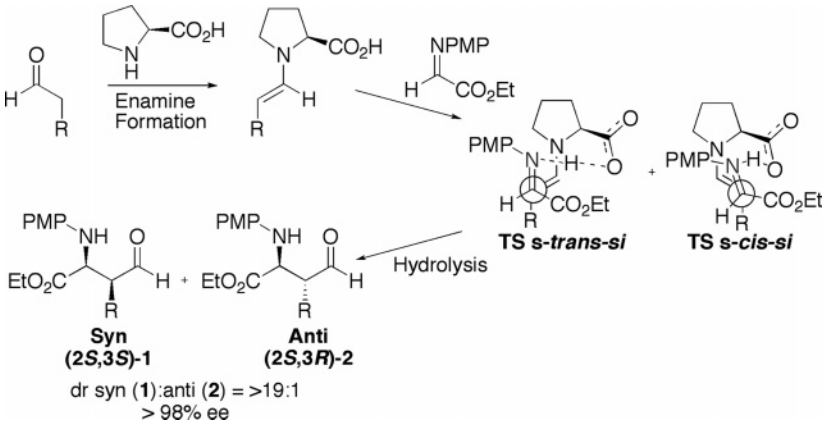
Scheme 1. Mechanism of the (*S*)-Proline-Catalyzed Mannich Reaction of Aldehydes with α-Imino Ethyl Glyoxylate



and *N*-*p*-methoxyphenyl (*N*-PMP)-protected α-imino ethyl glyoxylate.[4]

Pipecolic acid-catalyzed Mannich reactions provide both the *syn*-product **1** and the *anti*-product **2** in good yields (Table 1). The reaction rates were similar to that of proline-catalyzed reactions under the same conditions. The enantioselectivities of the *syn*-product (2*S*,3*S*)-**1**[4] and *anti*-product (2*S*,3*R*)-**2**[4,6] were both typically greater than 98% ee. The diastereomeric ratio of *syn*-product **1** to *anti*-product **2** ranged from 2:1 to 1:1, regardless of the bulkiness of the aldehyde substituent (Table 1). The insensitivity of the diastereoselectivity to steric bulk is in sharp contrast to the proline-catalyzed reactions, in which bulky R groups often led to excellent enantio- and diastereoselectivity.[4] (*S*)-Pipecolic acid catalysis provides a route to highly enantiomerically pure products of both diastereomers.

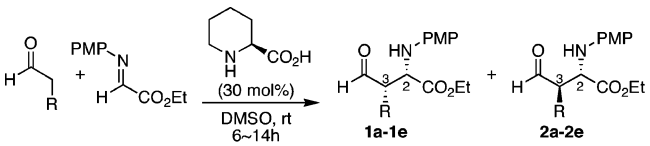
This unusual change in diastereoselectivity upon increase in the ring size of the catalyst caused us to investigate these reactions computationally. The enamine of propionaldehyde, *N*-PMP-protected α-imino methyl glyoxylate, and the transition structures leading to the four possible stereoisomeric products for both proline and pipecolic acid were calculated at the HF level of theory with the 6-31G(d) basis set.[7] We have previously used density functional theory to study related organocatalytic reactions.[8] However, HF/6-31G(d) was used over B3LYP/6-31G(d) in this study for rapidly computing the stereoselectivity.

The s-*cis*- or s-*trans*-enamine attack on the *re* or *si* face of the imine acceptor is the stereo- and rate-determining step of this reaction. Four possible diastereomeric transition structures are possible that allow for intramolecular proton transfer. The four lowest energy transition structures involving (*S*)-proline and (*S*)-pipecolic acid are shown in Figure 1.

The *syn*-product **1** arises from the s-*trans*-*si* transition state and the *anti*-product **2** from the s-*cis*-*si*. The conformations of the proline enamine were previously discussed as *anti*- and *syn*-enamine.[8] These notations are changed to s-*trans*- and s-*cis*-enamine, respectively, in this work to distinguish from *anti* and *syn* diastereoselective products. In the proline-catalyzed reaction, the computed energy difference between these transition structures, **TS-(*S*,*S*)-4** and **TS-(*R*,*S*)-6**, is 1.0 kcal/mol. The corresponding energy difference for the pipecolic acid-catalyzed reaction between **TS-(*S*,*S*)-8** and **TS-(*R*,*S*)-10** is only 0.2 kcal/mol. This decrease in energetic difference reflects the experimentally observed decrease in diastereoselectivity for the pipecolic acid-catalyzed reaction.

The computed selectivities arising from the relative energies for all transition structures are summarized in Table 2.

Table 1. (*S*)-Pipecolic Acid-Catalyzed Mannich Reaction of Aldehydes and α-Imino Ethyl Glyoxylate to Afford Products *syn*-**1a**−**e** and *anti*-**2a**−**e**[a]



Entry	R	Product	Yield (%)	dr *syn*(**1**):*anti*(**2**)	ee (%) *syn*(**1**)	ee (%) *anti*(**2**)
1	Me	**1a** + **2a**	80	2.0:1	>99	>99
2	*i*-Pr	**1b** + **2b**	82	1.4:1	>99	98
3	*n*-Bu	**1c** + **2c**	83	1.5:1	>99	>99
4	*n*-Pent	**1d** + **1d**	86	1.4:1	>99	>99
5		**1e** + **2e**	77	1.6:1	>99	99

[a] Typical conditions: To a solution of *N*-PMP-protected α-imino ethyl glyoxylate (0.5 mmol) and aldehyde (1.0 mmol) in anhydrous DMSO (5 mL) was added (*S*)-pipecolic acid (0.15 mmol), and the mixture was stirred for 6−14 h at room temperature. The diastereomeric ratio was determined without purification by ^{1}H NMR. The enantiomeric excess was determined by chiral-phase HPLC analysis.

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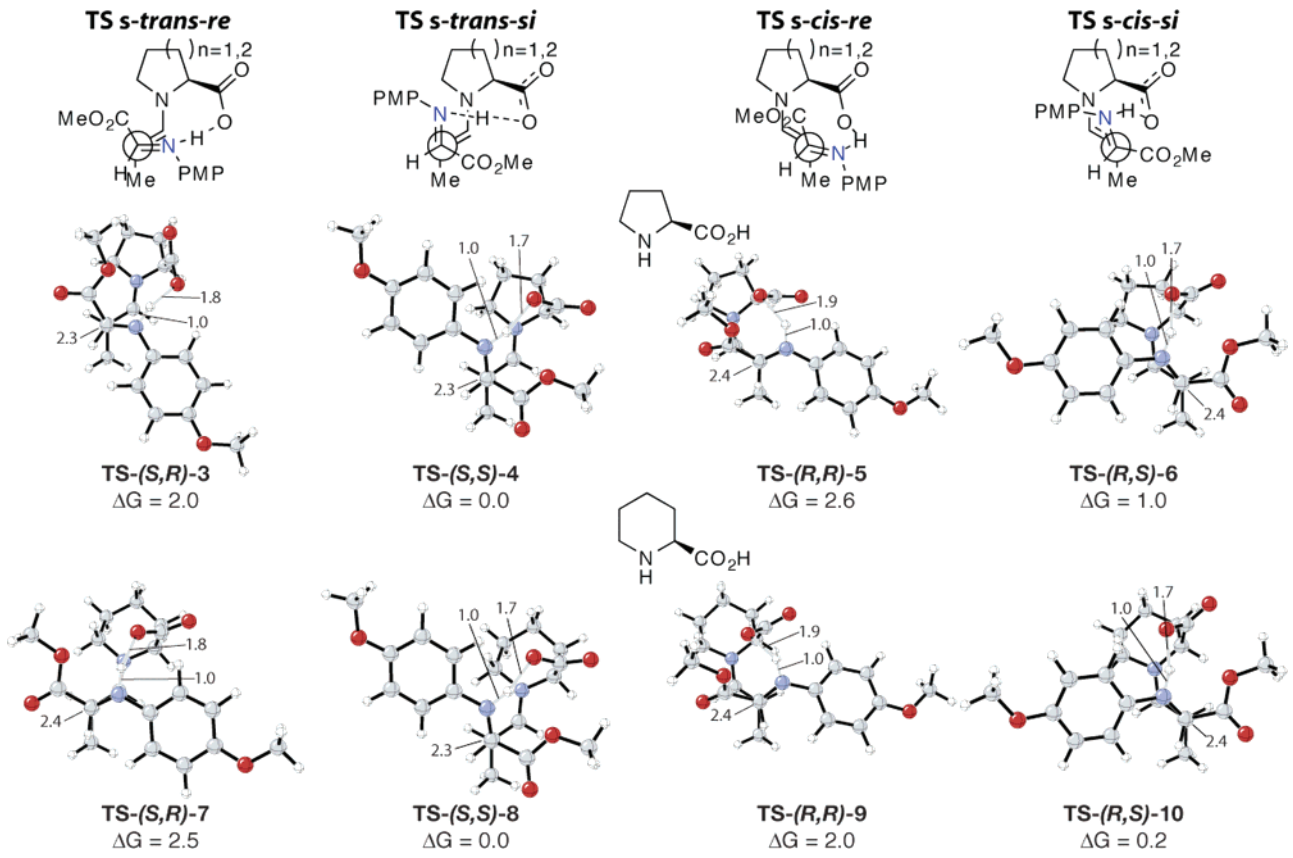

Figure 1. Transition structures for the C−C bond formation of the (*S*)-proline and (*S*)-pipecolic acid-catalyzed Mannich reaction between propionaldehyde and *N*-PMP-protected α-imino methyl glyoxylate; s-*trans*-*si* transition structures **TS-(*S*,*S*)-4** and **TS-(*S*,*S*)-8** give rise to product **1a**, while **TS-(*R*,*S*)-6** and **TS-(*R*,*S*)-10** gives rise to **2a**.

There is an excellent agreement between the computed stereoselectivity and the observed product ratios.

The facial *re* or *si* selectivity of the imine acceptor is governed by the necessity for intramolecular proton transfer and minimization of steric interactions between the imine and the reactive enamine. The (*E*)-imine is more stable than the (*Z*)-imine. Combined with the observation that transition structures involving intramolecular proton transfer are favored, the *re* face attacks necessitate substantial eclipsing of the imine and enamine [**TS-(*S*,*R*)-3**, **TS-(*S*,*R*)-7**, **TS-(*R*,*R*)-5**, and **TS-(*R*,*R*)-9**, Figure 1]. Consequently, as shown in Figure 1, the s-*trans*-*re* and s-*cis*-*re* transition structures are higher in energy by >1 kcal/mol than the s-*trans*-*si* or s-*cis*-*si* transition structure, for both proline and pipecolic acid.

Table 2. Comparison of the Experimentally Observed Product Ratios Involving Reaction of Propionaldehyde with *N*-PMP-Protected α-Imino Ethyl Glyoxylate with Computed Stereoselectivities Based on Transition State Theory Predictions Involving *N*-PMP-Protected α-Imino Methyl Glyoxylate

Entry	Catalyst	Type	dr *syn*(**1**):*anti*(**2**)	ee (%) *syn* (*anti*)
1	proline	exp.	3:1	>99
2	proline	computed	3.5:1	97
3	pipecolic acid	exp.	2:1	>99 (>99)
4	pipecolic acid	computed	1.4:1	93 (96)

The *re* or *si* attack on the enamine is determined by whether the s-*cis* or s-*trans* enamine conformer is favored in the transition state. In the case of proline, the transition structures involving the s-*trans*-enamine are favored over those that involve the s-*cis*-enamine. The latter involves distortions of the developing iminium from planarity to accommodate proton transfer. Thus proline provides the *syn*-product (2*S*,3*S*)-**1** as the major product.[8]

This differentiation is weakened in the case of pipecolic acid. The piperidine ring has steric interactions with the s-*trans*- or s-*cis*-enamines that are different than those of the pyrrolidine ring of proline. The relatively rigid piperidine ring holds the carboxylic acid more rigidly than the more flexible pyrrolidine. This alters electrostatic interactions with the ester of the iminoglyoxylate and with the protonated imine. These differences allow the imine to react via both the s-*trans*- and s-*cis*-enamine, giving rise to roughly equal amounts of both *syn*-product (2*S*,3*S*)-**1** and *anti*-product (2*S*,3*R*)-**2**.

The (*S*)-pipecolic acid-catalyzed Mannich reactions of aldehydes afford ready access to both syn- and *anti*-products

with high enantioselectivities. In contrast, proline-catalyzed reactions yield primarily the *syn*-product. Work is underway to further develop *anti*-selective Mannich catalysts based on these discoveries.[9,10]

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Supporting Information Available: Experimental procedures, characterization of compound, Cartesian coordinates, energies, thermodynamic corrections for all reported structures, full authorship of Gaussian and Q-Chem. This material is available free of charge via the Internet at http://pubs.acs.org.

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Supporting Information:
Pipecolic Acid-Catalyzed Asymmetric Mannich Reactions

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I. Experimental

General procedure for the pipecolic acid catalyzed asymmetric Mannich-type reaction between *N*-PMP protected α-imino ethyl glyoxylate and aldehyde donors: *N*-PMP-protected α-imino ethyl glyoxylate (0.5 mmol) was dissolved in anhydrous DMSO (5 mL) and the corresponding aldehyde donor (1.0 mmol) was added, followed by L-pipecolic acid (0.15 mmol). After stirring for overnight (6-14 h) at room temperature, the mixture was worked up by addition of saturated ammonium chloride solution and extraction with ethyl acetate (three or four times). The combined organic layers were washed with brine, dried with $MgSO_4$, filtered, and concentrated, and purified by flash column chromatography (10-20% EtOAc/hexanes) to afford the corresponding Mannich addition product. The enantiomeric excesses of all products were determined by chiral-phase HPLC analyses.

Ethyl 3-formyl-2-(*p*-methoxyphenylamino)butenoate (1a + 2a): data were described previously. [S1]

Ethyl 3-formyl-2-(*p*-methoxyphenylamino)-4-methyl-pentanoate (1b + 2b): ^{1}H NMR (500 MHz, $CDCl_3$): purified 1:1 mixture of diasteromers, * denotes *anti*-diasteromer (**2b**), δ = 1.03 (d, 3H x 1/2, *J* = 6.6 Hz, CHCH_3), 1.08 (d, 3H* x 1/2, *J* = 7

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(S1) Cordova, A.; Watanabe, S.; Tanaka, F.; Notz, W.; Barbas, C. F., III *J. Am. Chem. Soc.* **2002**, *124*, 1866.

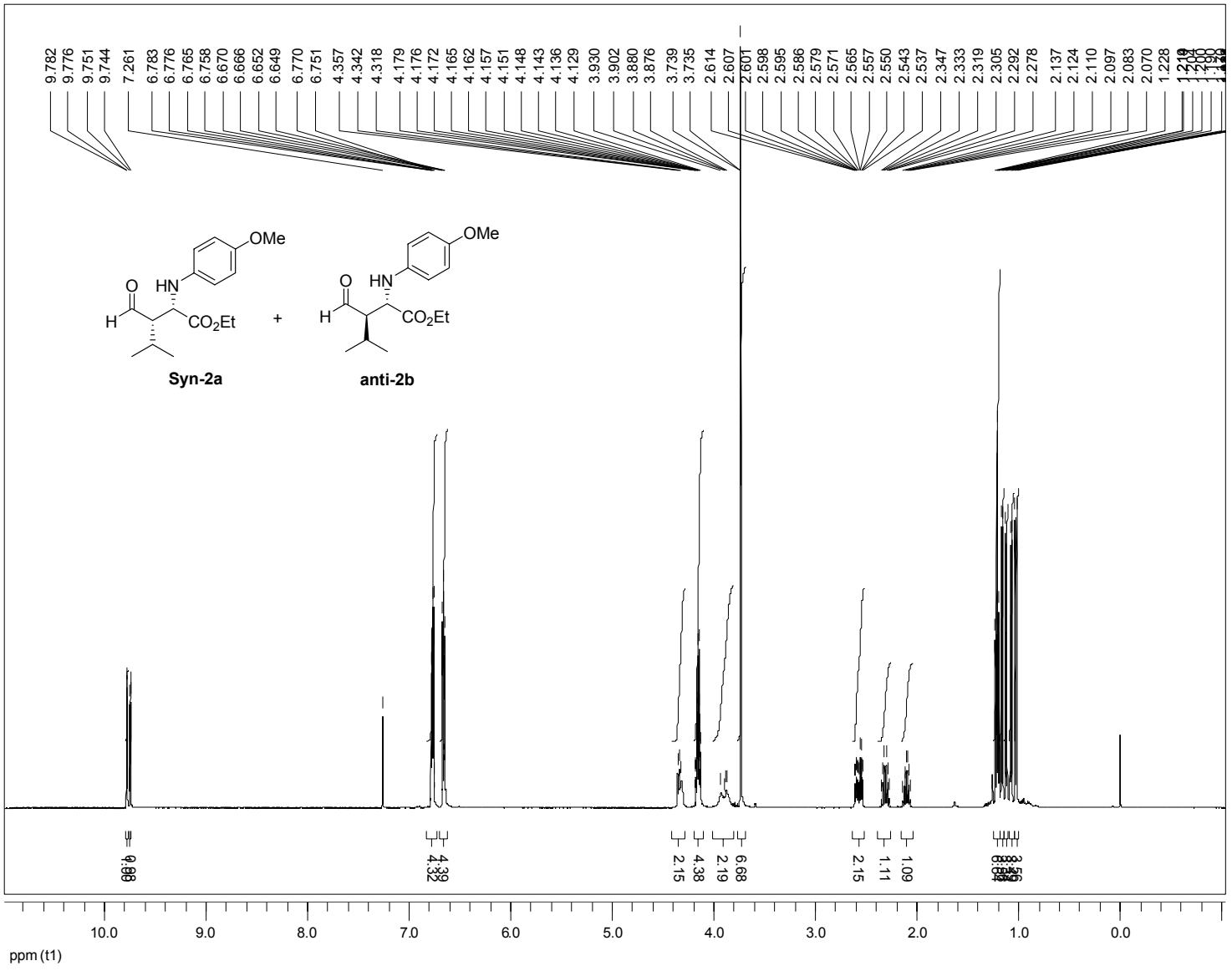
Hz, OCHC*H*$_3$), 1.12 (d, 3H* x 1/2, *J* = 7 Hz, CHC*H*$_3$), 1.16 (d, 3H x 1/2, *J* = 6.6 Hz, CHC*H*$_3$), 1.22 (t, 3H, OCH$_2$C*H*$_3$), 2.13 (m, 1H* x 1/2, C*H*(CH$_3$)$_2$), 2.34 (m, 1H x 1/2, C*H*(CH$_3$)$_2$), 2.54-2.61 (m, 1H, C*H*CHO), 3.74 (s, 3H, OC*H*$_3$), 3.93-3.87 (1H, N*H*), 4.17-4.12 (m, 2H, OC*H*$_2$CH$_3$), 4.35-4.31 (m, 1H, C*H*NHPMP), 6.64 (m, 2H, Ar*H*), 6.78 (m, 2H, Ar*H*), 9.75 (d, 1H* x 1/2, *J* = 3.5 Hz, CHC*H*O), 9.78 (d, 1H x 1/2, *J* = 3.0 Hz, CHC*H*O); ^{13}C NMR (125 MHz, $CDCl_3$): mixture of diasteromers, δ = 203.6, 203.2, 172.8, 172.6, 153.3, 153.1, 140.4, 140.1, 115.9, 114.8, 114.7, 61.4, 59.6, 59.5, 57.2, 57.0, 55.6, 27.5, 26.3, 21.2, 20.9, 19.8, 19.2, 14.1; HPLC (Daicel Chairalcel AS-H, hexane /*i*-PrOH = 99:1, 1.0 mL/min, λ = 254 nm) t_R (*syn* major enantiomer, (2*S*,3*S*)-**1b**) = 30.3 min; t_R (*syn* minor enantiomer, (2*R*,3*R*) **1b**) = 57.1 min; t_R (*anti* major enantiomer, (2*S*,3*R*)-**2b**) = 23.1 min; t_R (*anti* minor enantiomer, (2*R*,3*S*)-**2b**) = 51.1 min. HRMS: calcd for $C_{16}H_{23}NO_4$ (MNa^+) 316.1519, found: 316.1521.

Ethyl 3-formyl-2-(*p*-methoxyphenylamino)heptanoate (1c + 2c): ^{1}H NMR (300 MHz, $CDCl_3$): purified 1.5:1 mixture of diasteromers, * denotes *anti*-diasteromer (**2c**), δ = 0.89-1.02 (m, 3H), 1.23 (t, 3H* x 2/5, *J* = 7.1 Hz), 1.24 (t, 3H x 3/5, *J* = 7.1 Hz), 1.28-1.90 (m, 6H), 2.68-2.78 (m, 1H), 3.73 (s, 3H), 3.89 (brd, 1H x 3/5, *J* = 10.2 Hz), 4.03 (brd, 1H* x 2/5, *J* = 10.2 Hz), 4.18 (m, 2H), 4.26 (m, 1H* x 2/5), 4.35 (dd, 1H x 3/5, *J* = 5.0 Hz, 10.2 Hz), 6.65 (d, 2H, *J* = 8.1 Hz), 6.77 (d, 2H, *J* = 8.1 Hz), 9.65 (d, 1H* x 2/5, *J* = 2.4 Hz), 9.71 (d, 1H x 3/5, *J* = 2.1 Hz); ^{13}C NMR (75 MHz, $CDCl_3$): δ = 202.9, 202.8, 172.4, 172.2, 153.3, 153.1, 140.4, 140.3, 116.1, 115.7, 114.8, 114.8, 61.5, 61.5, 58.4, 58.1, 55.6, 53.9, 53.7, 29.6, 29.4, 25.4, 24.8, 22.6, 14.1, 13.8 (for ^{13}C NMR hard copy, see ref S1); HPLC (Daicel Chiralpak AS-H, hexane/*i*-PrOH = 99:1, flow rate 1.0 mL/min, λ = 254 nm); t_R (*syn* major enantiomer, (2*S*,3*S*)-**1c**) = 35.3 min; t_R (*syn* minor enantiomer, (2*R*,3*R*)-**1c**) = 54.2 min; t_R (*anti* major enantiomer, (2*S*,3*R*)-**2c**) = 27.4 min; t_R (*anti* minor enantiomer, (2*R*,3*S*)-**2c**) = 32.8 min. HRMS: Calcd for $C_{17}H_{25}NO_4$ (MNa^+): 307.1778, found: 307.1781.

Ethyl 3-formyl-2-(*p*-methoxyphenylamino)octanoate (1d + 2d): ^{1}H NMR (500 MHz, $CDCl_3$): purified 1.5:1 mixture of diasteromers, * denotes *anti*-diasteromer (**2d**), δ = 0.89 (m, 3H), 1.24 (t, 3H, *J* = 7.1 Hz), 1.25-1.90 (m, 8H), 2.76 (m, 1H), 3.73 (s, 3H), 3.95-4.10 (1H), 4.14-4.20 (m, 2H), 4.26 (m, 1H* x 2/5), 4.37 (m, 1H x 3/5), 6.65 (m, 2H), 6.78 (m, 2H), 9.65 (d, 1H* x 2/5, *J* = 2.0 Hz), 9.71 (d, 1H x 3/5, *J* = 1.5 Hz); ^{13}C

NMR (120 MHz, $CDCl_3$): δ = 202.6, 202.2, 172.2, 153.3, 153.1, 140.5, 140.3, 116.0, 115.7, 114.8, 61.5, 58.4, 58.1, 57.2, 55.6, 53.9, 53.7, 31.6, 27.1 26.9, 25.6, 22.5, 22.3, 14.1, 13.9; HPLC (Daicel Chairalcel AS-H, hexane/*i*-PrOH =99:1, 1.0 mL/min, λ = 254 nm) t_R (*syn* major enantiomer, (2*S*,3*S*)-**1d**) = 24.9 min; t_R (*syn* minor enantiomer, (2*R*,3*R*)-**1d**) = 34.8 min; t_R (*anti* major enantiomer, (2*S*,3*R*)-**2d**) = 21.1 min; t_R (*anti* minor enantiomer (2*R*,3*S*)-**2d**) = 23.2 min. HRMS: Calcd for $C_{18}H_{27}NO_4$ (MH^+) 322.2013, found: 322.2021.

Ethyl 3-formyl-2-(*p*-methoxyphenylamino)hex-5-enoate (1e + 2e): ^{1}H NMR (400 MHz, $CDCl_3$): 1.6:1 mixture of diastereomers, * denotes *anti*-diasteromer (**2e**), δ = 1.23 (t, 3H* x 5/13, *J* = 7.2 Hz, OCHC*H*$_3$), 1.24 (t, 3H x 8/13, *J* = 7.2 Hz, OCHC*H*$_3$), 2.42-2.70 (m, 2H, C*H*$_2$CH=CH$_2$), 2.86-2.88 (m, 1H x 8/13, C*H*CHO), 2.96-2.97(m, 1H* x 5/13, C*H*CHO), 3.73 (s, 3H, OC*H*$_3$), 4.00 (d, 1H x 8/13, *J* = 9.6Hz, N*H*), 4.07 (d, 1H* x 5/13, *J* = 9.6Hz, N*H*), 4.15-4.20 (m, 2H, OC*H*$_2$CH$_3$), 4.26-4.30 (m, 1H* x 5/13, C*H*NHPMP), 4.36-4.39 (m, 1H x 8/13, C*H*NHPMP), 5.13-5.19 (m, 2H, CH=C*H*$_2$), 5.77-5.88 (m, 1H, C*H*=CH$_2$), 6.64-6.78 (m, 4H, Ar*H*), 9.68 (d, 1H* x 5/13, *J* = 1.6 Hz , CHC*H*O), 9.72 (d, 1H x 8/13, *J* = 1.2 Hz, CHC*H*O); ^{13}C NMR (100 MHz, $CDCl_3$): 201.9, 172.2, 172.2, 153.3, 153.1, 140.5, 140.3, 134.3, 118.2, 116.1, 115.8, 114.8, 61.6, 57.8, 57.7, 55.6, 53.1, 53.0, 30.0, 29.7, 14.1. HPLC (Daicel Chairalcel AS-H, hexane /*i*-PrOH =99:1, 1.0 mL/min, λ = 254 nm) t_R (*syn* major enantiomer, (2*S*,3*S*)-**1e**) = 45.5 min; t_R (*syn* minor enantiomer, (2*R*,3*R*)-**1e**) = 80.1 min; t_R (*anti* major enantiomer (2*S*,3*R*)-**2e**) = 33.9 min; t_R (*anti* minor enantiomer (2*R*,3*S*)-**2e**) = 42.7 min. HRMS: Calcd for $C_{16}H_{22}NO_4$ (MH^+) 292.1543, found: 292.1537.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CO2Et
+
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anti-2b
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4.38
2.19
6.68
2.15
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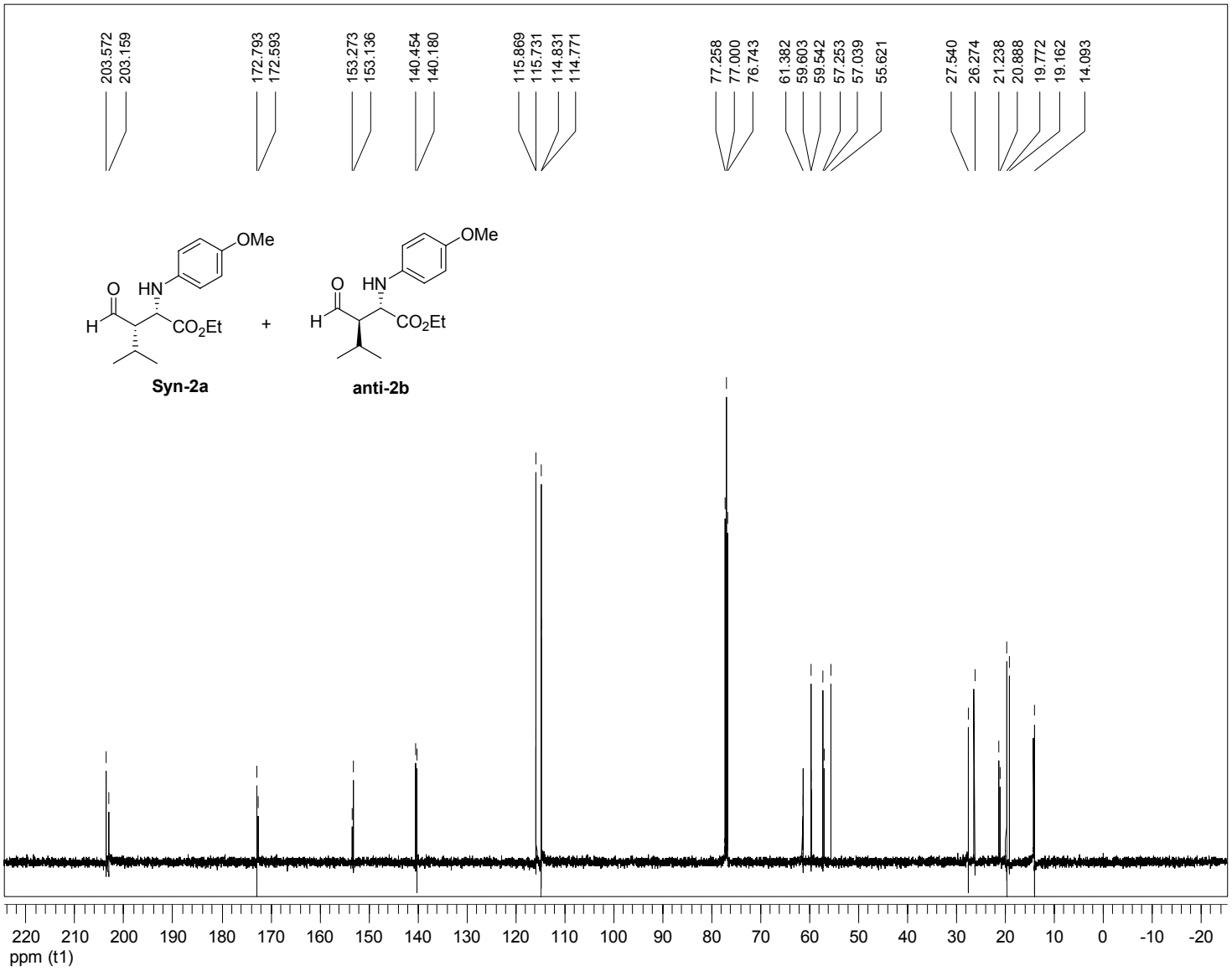
ppm (t1)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HN
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H
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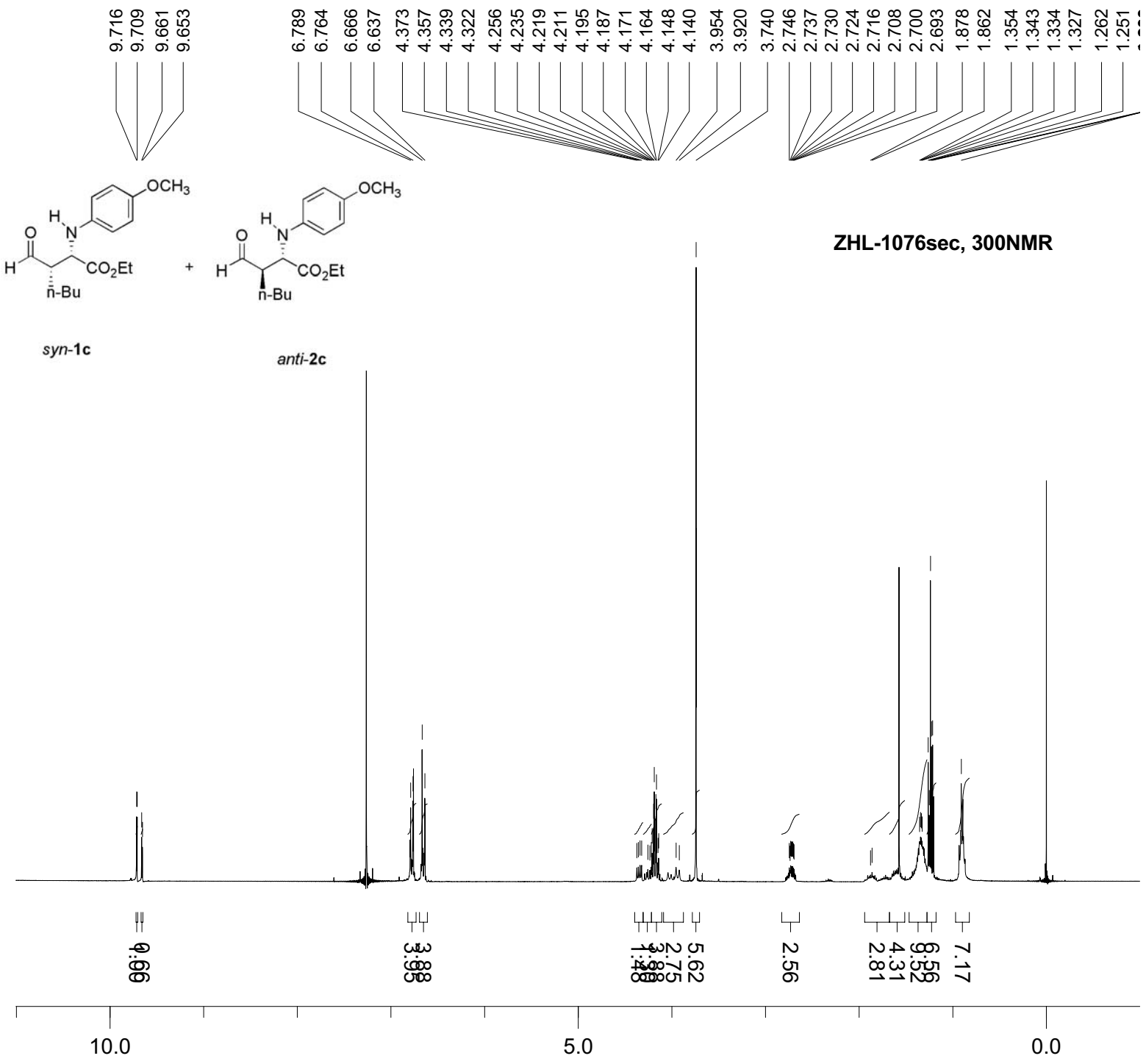

Date:
15 Aug 2005
Document's Title:
ZHL-1076forOL.mrc

Spectrum Title:
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Actual Points Count:
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Acquisition Time (sec):
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Spectral Width (ppm):
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Pulse Program:
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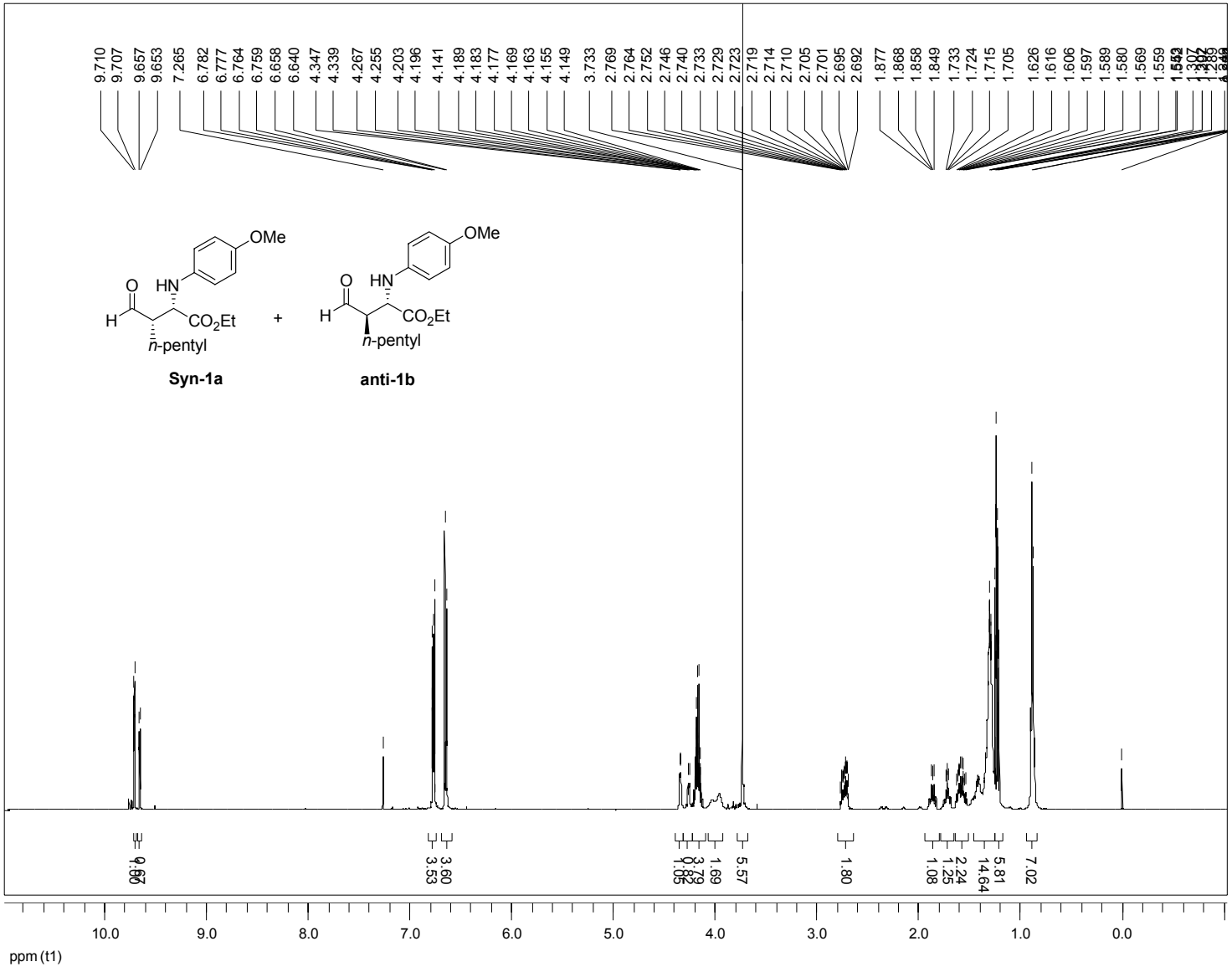
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4.267
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4.196
4.141
4.189
4.183
4.177
4.169
4.163
4.155
4.149
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2.764
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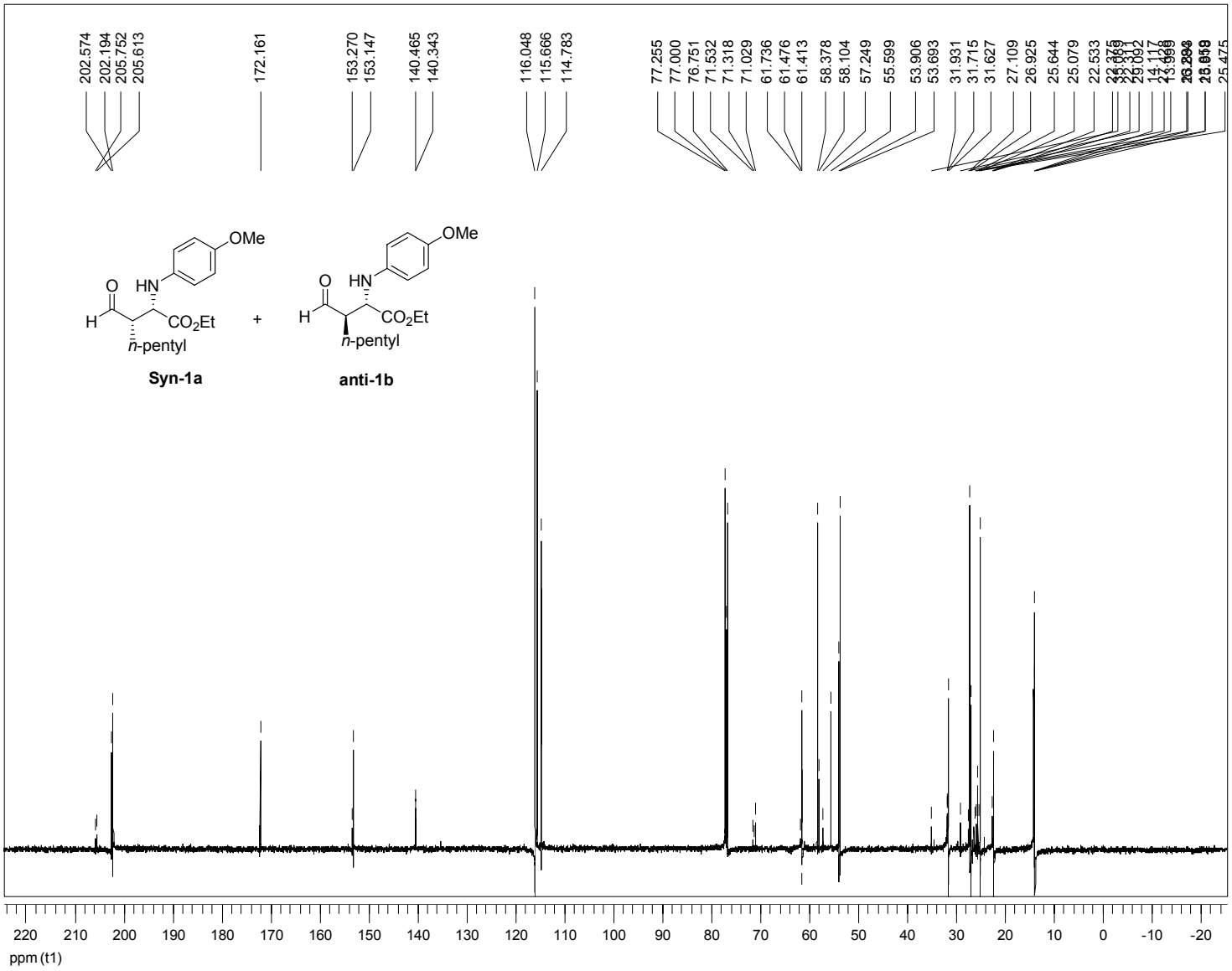
ppm (t1)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H
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anti-1b
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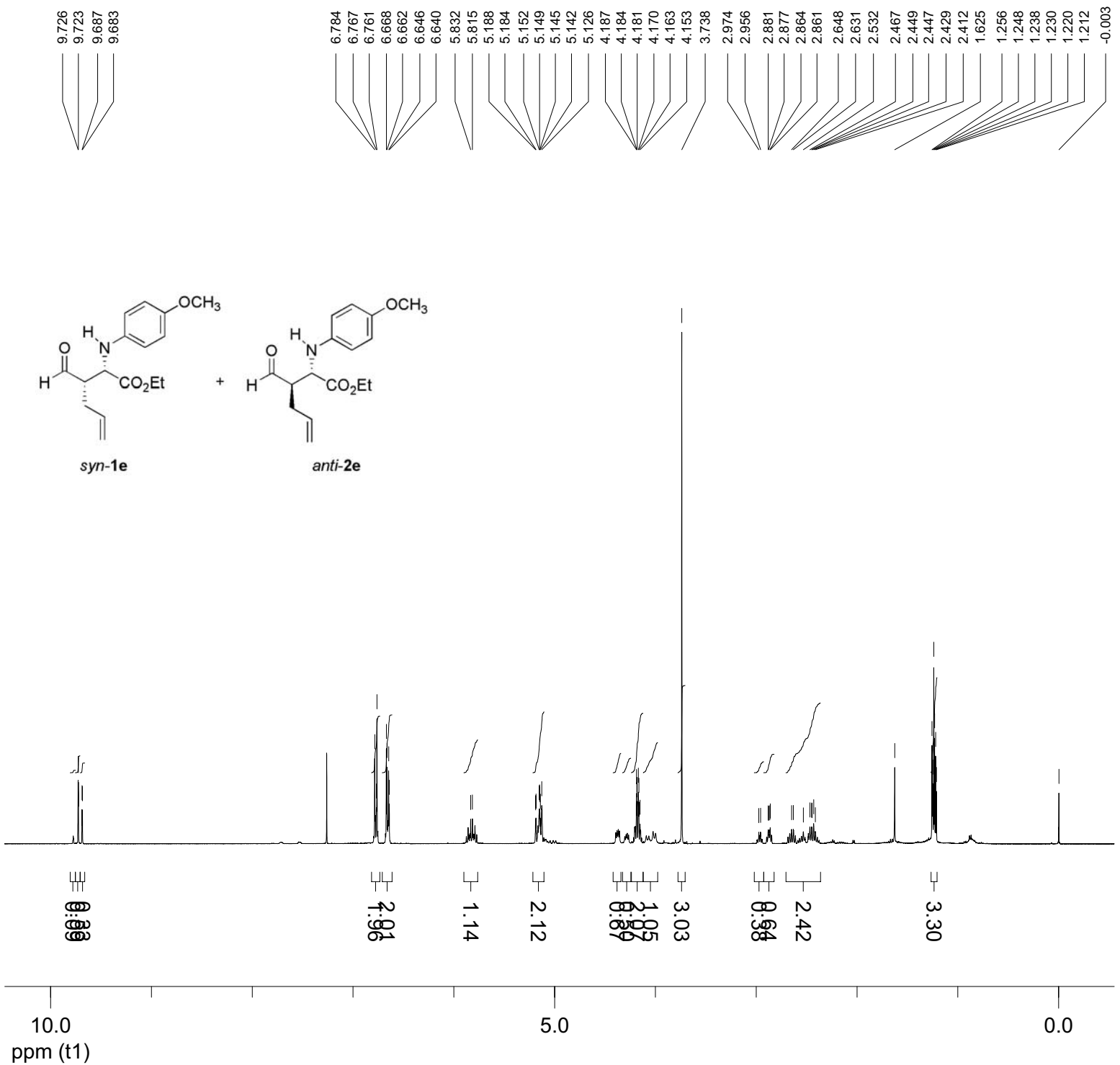

Date:
15 Aug 2005
Document's Title:
ZHL-1121-b2-b3.mrc

Spectrum Title:
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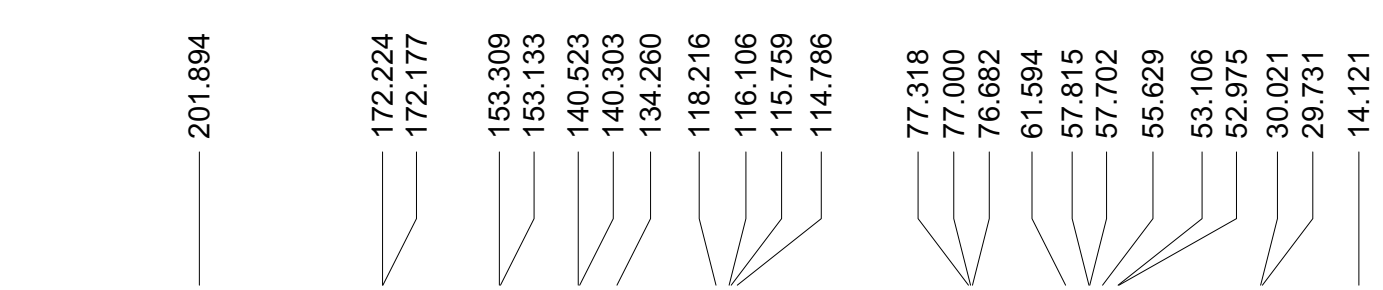
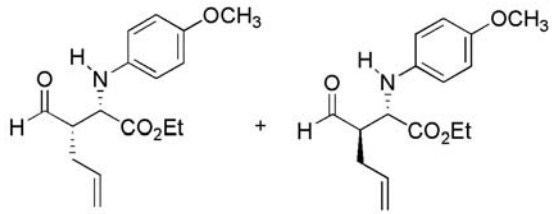
Acq. Date:
Jul 15 2005



400 CNMR, ZHL-1121-b4-b7-car



syn-**1e** + *anti*-**2e**

Date:
15 Aug 2005
Document's Title:
parameterZHL-1121-b4-b7car.mrc

Spectrum Title:
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Actual Points Count:
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Spectral Width (ppm):
(f1) 249.945
Pulse Program:
Unknown
Temperature:
29

Number of Scans:
512

Acq. Date:
Jul 16 2005

II. Computational Supporting Information

A. Authors of Computational Packages

Authors of Q-Chem 3.1:
J. Kong, C. A. White, A. I. Krylov, C. D. Sherrill,
R. D. Adamson, T. R. Furlani, M. S. Lee, A. M. Lee,
S. R. Gwaltney, T. R. Adams, C. Ochsenfeld, A. T. B. Gilbert,
G. S. Kedziora, V. A. Rassolov, D. R. Maurice, N. Nair,
Y. Shao, N. A. Besley, P. E. Maslen, J. P. Dombroski,
H. Dachsel, W. M. Zhang, P. P. Korambath, J. Baker,
E. F. C. Byrd, T. Van Voorhis, M. Oumi, S. Hirata,
C. P. Hsu, N. Ishikawa, J. Florian, A. Warshel,
B. G. Johnson, P. M. W. Gill, M. Head-Gordon, J. A. Pople,
Q-Chem, Version 2.0, Q-Chem, Inc., Export, PA (2000).

Authors of Gaussian 03:
Gaussian 03, Revision C.01,
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria,
M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven,
K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi,
V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega,
G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota,
R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao,
H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross,
C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev,
A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala,
K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg,
V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain,
O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari,
J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford,
J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz,
I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham,
C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill,
B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople,
Gaussian, Inc., Wallingford CT, 2004.

B. Relevant geometries, energies, thermodynamic data, frequencies, and Gaussian route section of structures.

i. Proline

Supporting Information: s-Trans-Re-3D-(Methyl-Syn)-(Esther-Anti).output

Using Gaussian 03: Al64T-G03RevC.01 3-Apr-2004

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Pointgroup= C1 Stoichiometry= C18H24N2O5 C1[X(C18H24N2O5)] #Atoms= 49
Charge = 0 Multiplicity = 1

SCF Energy= -1178.72703201 Predicted Change= -4.224142D-08

Optimization completed. {Found 1 times}

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C	-1.257931	-0.282739	1.497454
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C	-0.106644	1.643379	-0.269540
C	0.028003	1.473290	2.746924
N	0.594674	0.700111	-0.806472
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C	4.193147	1.243911	-0.091004
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C	1.969555	0.459035	-0.532779
C	2.423500	-0.846650	-0.498104
C	3.763346	-1.112005	-0.249855
O	5.965670	-0.221664	0.214457
C	6.524617	-1.506123	0.251542
C	-1.454355	1.956136	-0.847085
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O	-2.065718	1.218089	-1.539796
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C	-1.595945	-2.302359	-0.890080

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Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

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SCF Energy= -1178.72703201 Predicted Change= -4.224142D-08
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Internal Energy (U)= -1178.2662 0.46077
Enthalpy (H)= -1178.2653 0.46172
Gibbs Free Energy (G)= -1178.3447 0.38232

Frequencies -- -318.6211 28.3273 29.6629

Supporting Information: s-Trans-Re-3D-(Methyl-Syn)-(Esther-Syn).output

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Using Gaussian 03: Al64T-G03RevC.01 3-Apr-2004

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Pointgroup= C1 Stoichiometry= C18H24N2O5 C1[X(C18H24N2O5)] #Atoms= 49
Charge = 0 Multiplicity = 1

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C	-4.553590	-1.032645	0.641028
C	-3.847858	-2.391428	0.618351
C	-2.376070	-2.031259	0.461030
C	-1.125213	-0.237880	1.574522
C	-0.859782	1.054619	1.987322
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C	0.363495	1.341077	2.834065
N	0.631483	0.799045	-0.734637
C	4.664874	-0.188391	-0.099766
C	4.266135	1.147299	-0.083968
C	2.949158	1.483427	-0.295636
C	1.998826	0.488187	-0.505203
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 Temperature= 298.150 Kelvin       Pressure= 1.00000 Atm
================================================================================
 SCF Energy=     -1178.73180651         Predicted Change= -2.397847D-08
 Zero-point correction (ZPE)=      -1178.2939      0.43783
 Internal Energy (U)=                      -1178.2705      0.46123
 Enthalpy (H)=                             -1178.2696       0.46217
 Gibbs Free Energy (G)=                    -1178.3476       0.38413
--------------------------------------------------------------------------------
 Frequencies --  -359.9596               30.2640               35.2485

 Supporting Information: s-Trans-Re-3U-(Methyl-Anti)-(Esther-Anti).output
--------------------------------------------------------------------------------
 Using  Gaussian 03:  Al64T-G03RevC.01  3-Apr-2004
================================================================================
 # opt=(calcfc,ts,maxcycle=150,noeigentest) freq=noraman hf/6-31g(d)
 geom=connectivity scf=(direct,tight,maxcycle=300)
 #N Geom=AllCheck Guess=Read SCRF=Check GenChk RHF/6-31G(d) Freq
--------------------------------------------------------------------------------
 Pointgroup= C1   Stoichiometry= C18H24N2O5   C1[X(C18H24N2O5)]  #Atoms= 49
 Charge = 0         Multiplicity = 1
--------------------------------------------------------------------------------
 SCF Energy= -1178.72599682   Predicted Change= -8.664731D-08
================================================================================
 Optimization completed.           {Found        1        times}
 Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force      0.00005 ||  0.00045   [ YES ]      0.00000 ||  0.00030   [ YES ]
 Displ      0.00527 ||  0.00180   [ NO ]       0.00527 ||  0.00180   [ YES ]
--------------------------------------------------------------------------------
      Atomic             Coordinates (Angstroms)
       Type           X             Y         Z
--------------------------------------------------------------------------------
       N        -2.478103      -0.998102       0.883540
       C        -3.804374      -0.397913       0.744714
       C        -4.663470      -1.559366       0.245728
       C        -3.673706      -2.390693      -0.574753
       C        -2.386873      -2.335612       0.243521
       C        -1.435669      -0.406498       1.411720
       C        -1.286653       0.924183       1.778154
       C        -0.188141       1.553627      -0.180686
       C        -0.231310       1.305129       2.797168
       N         0.451964       0.617738      -0.817353
       C         4.464231      -0.393147      -0.070679
       C         4.088738       0.939452      -0.134435
       C         2.763801       1.266230      -0.390053
       C         1.812130       0.279106      -0.557104
       C         2.190597      -1.062490      -0.513352
       C         3.506162      -1.385305      -0.268886
       O         5.717966      -0.822332       0.165838
       C         6.748193       0.104609       0.356025
       C        -1.456681       2.097034      -0.771332
       O        -1.700151       3.299532      -0.288569
       O        -2.107677       1.541682      -1.587273
       C        -2.857970       3.965040      -0.775478
       C        -1.072667      -2.423533      -0.573481
       O        -0.978329      -1.608849      -1.508657
       O        -0.244116      -3.222330      -0.163260
       H        -3.777911       0.401884       0.016899
       H        -4.133357       0.005044       1.695989
       H        -5.038267      -2.134555       1.086984
       H        -5.514552      -1.214489      -0.329308
       H        -4.005105      -3.409456      -0.734532
       H        -3.493291      -1.927092      -1.536328
       H        -2.376142      -3.092828       1.018010
       H        -0.571808      -1.045461       1.495850
       H        -2.171964       1.539072       1.783691
       H         0.371214       2.224234       0.435503
       H         0.667586       0.706545       2.683160
       H         0.052687       2.349682       2.699572
       H        -0.583212       1.173718       3.817923
       H        -0.098690      -0.076301      -1.335242
       H         4.803379       1.729090      -0.010064
       H         2.496077       2.304029      -0.480455
       H         1.464845      -1.842414      -0.659165
       H         3.812807      -2.413156      -0.224732
       H         6.886007       0.729457      -0.520219
       H         6.561467       0.733217       1.220618
       H         7.645003      -0.471971       0.524548
       H        -3.746594       3.408356      -0.515545
       H        -2.863996       4.929219      -0.293906
       H        -2.802780       4.075986      -1.847922
--------------------------------------------------------------------------------
 Statistical Thermodynamic Analysis
 Temperature= 298.150 Kelvin       Pressure= 1.00000 Atm
================================================================================
 SCF Energy=     -1178.72599682         Predicted Change= -8.664731D-08
 Zero-point correction (ZPE)=      -1178.2884      0.43757
 Internal Energy (U)=                      -1178.2648      0.46111
 Enthalpy (H)=                             -1178.2639       0.46205
 Gibbs Free Energy (G)=                    -1178.3429       0.38303
--------------------------------------------------------------------------------
 Frequencies --  -353.2953               25.0887               36.4296

 Supporting Information: s-Trans-Re-3U-(Methyl-Anti)-(Esther-Syn).output
--------------------------------------------------------------------------------
 Using  Gaussian 03:  Al64T-G03RevC.01  3-Apr-2004
================================================================================
 #hf/6-31g* scf=(direct,tight,maxcycle=300)
 opt=(calcfc,maxcycle=150,ts,noeigentest) freq=noraman
 #N Geom=AllCheck Guess=Read SCRF=Check GenChk RHF/6-31G(d) Freq
--------------------------------------------------------------------------------
 Pointgroup= C1   Stoichiometry= C18H24N2O5   C1[X(C18H24N2O5)]  #Atoms= 49
 Charge = 0         Multiplicity = 1
```

```
 ---------------------------------------------------------------------------
 SCF Energy= -1178.72658857   Predicted Change= -7.524670D-09
 ===========================================================================
 Optimization completed.            {Found       2        times}
 Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force      0.00001 ||  0.00045   [ YES ]      0.00000 ||  0.00030   [ YES ]
 Displ      0.00080 ||  0.00180   [ YES ]      0.00080 ||  0.00180   [ YES ]
 ---------------------------------------------------------------------------
      Atomic             Coordinates (Angstroms)
       Type           X             Y         Z
 ---------------------------------------------------------------------------
       N        -2.472152      -1.157933       0.899739
       C        -3.744743      -0.592153       1.341800
       C        -4.767041      -1.456311       0.606429
       C        -4.063645      -1.765696      -0.718898
       C        -2.603954      -1.987412      -0.319589
       C        -1.284617      -0.846654       1.376889
       C        -0.920336       0.194423       2.205319
       C        -0.145608       1.491397       0.438044
       C         0.338038       0.087723       3.040344
       N         0.532980       0.859165      -0.478099
       C         4.504006      -0.479687      -0.241888
       C         4.170391       0.763139       0.272881
       C         2.858957       1.213030       0.191530
       C         1.879986       0.423694      -0.376865
       C         2.215241      -0.821400      -0.907291
       C         3.516735      -1.262693      -0.837641
       O         5.741774      -1.008746      -0.220342
       C         6.799885      -0.285063       0.340549
       C        -1.442222       2.165565       0.010312
       O        -1.341227       2.586955      -1.220499
       O        -2.358395       2.366228       0.734685
       C        -2.523001       3.076236      -1.842404
       C        -1.552821      -1.509609      -1.348498
       O        -1.628611      -0.299338      -1.648657
       O        -0.704060      -2.321837      -1.681024
       H        -3.825182       0.445861       1.051950
       H        -3.822285      -0.654270       2.421213
       H        -4.950935      -2.371700       1.160848
       H        -5.714874      -0.946790       0.478279
       H        -4.476577      -2.626953      -1.229659
       H        -4.121926      -0.911761      -1.382556
       H        -2.413479      -3.024575      -0.071185
       H        -0.494214      -1.475972       1.000058
       H        -1.697180       0.825746       2.596958
       H         0.383657       1.969933       1.235610
       H         1.100679      -0.506880       2.547906
       H         0.766240       1.065379       3.249900
       H         0.138367      -0.372079       4.005513
       H        -0.039562       0.460655      -1.224120
       H         4.909164       1.398213       0.720739
       H         2.623797       2.194690       0.562262
       H         1.453432      -1.431322      -1.362680
       H         3.792032      -2.219679      -1.238926
       H         6.963031       0.649822      -0.185269
       H         6.627202      -0.081505       1.392262
       H         7.676686      -0.906329       0.239316
       H        -2.919672       3.914701      -1.289938
       H        -2.222482       3.378625      -2.831743
       H        -3.249072       2.280299      -1.897647
 ---------------------------------------------------------------------------
 Statistical Thermodynamic Analysis
 Temperature= 298.150 Kelvin       Pressure= 1.00000 Atm
 ===========================================================================
 SCF Energy=     -1178.72658857         Predicted Change= -7.524670D-09
 Zero-point correction (ZPE)=      -1178.2887      0.43786
 Internal Energy (U)=                      -1178.2652      0.46130
 Enthalpy (H)=                             -1178.2643       0.46224
 Gibbs Free Energy (G)=                    -1178.3430       0.38352
 ---------------------------------------------------------------------------
 Frequencies --  -380.4655               28.2735               36.5807

 Supporting Information: s-Trans-Re-3U-(Methyl-Syn)-(Esther-Anti).output
 ---------------------------------------------------------------------------
 Using  Gaussian 03:  IA32L-G03RevC.02 12-Jun-2004
 ===========================================================================
 # opt=(calcfc,ts,maxcycle=150,noeigentest) freq=noraman hf/6-31g(d)
 geom=connectivity scf=(direct,tight,maxcycle=300)
 #N Geom=AllCheck Guess=Read SCRF=Check GenChk RHF/6-31G(d) Freq
 ---------------------------------------------------------------------------
 Pointgroup= C1   Stoichiometry= C18H24N2O5   C1[X(C18H24N2O5)]  #Atoms= 49
 Charge = 0         Multiplicity = 1
 ---------------------------------------------------------------------------
 SCF Energy= -1178.72745322   Predicted Change= -4.261283D-09
 ===========================================================================
 Optimization completed.            {Found       2        times}
 Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force      0.00002 ||  0.00045   [ YES ]      0.00000 ||  0.00030   [ YES ]
 Displ      0.00139 ||  0.00180   [ YES ]      0.00139 ||  0.00180   [ YES ]
 ---------------------------------------------------------------------------
      Atomic             Coordinates (Angstroms)
       Type           X             Y         Z
 ---------------------------------------------------------------------------
       N        -2.310596      -1.184266       0.869085
       C        -3.700839      -0.755343       0.723134
       C        -4.407564      -2.020930       0.239339
       C        -3.322636      -2.728636      -0.576573
       C        -2.049097      -2.500601       0.233982
       C        -1.354071      -0.466598       1.403220
       C        -1.377416       0.870759       1.775329
       C        -0.363417       1.651389      -0.171175
       C        -0.384703       1.378010       2.802388
       N         0.385713       0.805880      -0.814996
       C         4.472284       0.204999      -0.026393
       C         3.943248       1.494762      -0.032232
       C         2.608617       1.694155      -0.297404
```

C	1.770195	0.608436	-0.539829
C	2.293258	-0.671618	-0.555502
C	3.643276	-0.871276	-0.296371
O	5.788219	0.113266	0.240571
C	6.409733	-1.142574	0.241979
C	-1.685779	2.042575	-0.764102
O	-2.078688	3.199380	-0.269368
O	-2.258811	1.420378	-1.590439
C	-3.307066	3.723042	-0.756836
C	-0.743448	-2.426905	-0.598146
O	-0.750957	-1.585330	-1.514161
O	0.169801	-3.146475	-0.223216
H	-3.772591	0.032496	-0.014757
H	-4.078766	-0.384840	1.669339
H	-4.704374	-2.629968	1.087882
H	-5.296790	-1.792689	-0.336092
H	-3.521624	-3.783052	-0.723965
H	-3.207487	-2.256516	-1.544089
H	-1.934772	-3.246497	1.011109
H	-0.416200	-0.990658	1.490247
H	-2.334474	1.366647	1.779888
H	0.107774	2.378806	0.454034
H	0.584289	0.900679	2.690613
H	-0.236521	2.450853	2.711744
H	-0.722092	1.196865	3.820418
H	-0.079107	0.060076	-1.342564
H	4.600080	2.323581	0.153655
H	2.228700	2.699460	-0.338938
H	1.663879	-1.519469	-0.755616
H	4.017907	-1.875631	-0.307177
H	5.984199	-1.793247	0.998037
H	6.335037	-1.621136	-0.728262
H	7.449120	-0.962709	0.471329
H	-4.121580	3.057776	-0.509651
H	-3.434614	4.673117	-0.264265
H	-3.259786	3.853121	-1.827491

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

SCF Energy= -1178.72745322 Predicted Change= -4.261283D-09
Zero-point correction (ZPE)= -1178.2898 0.43764
Internal Energy (U)= -1178.2662 0.46120
Enthalpy (H)= -1178.2653 0.46214
Gibbs Free Energy (G)= -1178.3444 0.38301

Frequencies -- -357.7627 24.4570 34.6059

Supporting Information: s-Trans-Re-3U-(Methyl-Syn)-(Esther-Syn).output

---

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

---

opt=(calcfc,ts,maxcycle=150,noeigentest) freq=noraman hf/6-31g(d)

geom=connectivity scf=(direct,tight,maxcycle=300)
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RHF/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C18H24N2O5 C1[X(C18H24N2O5)] #Atoms= 49
Charge = 0 Multiplicity = 1

SCF Energy= -1178.72758451 Predicted Change= -3.552982D-08

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00002	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00230	0.00180	[NO]	0.00230	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
N	-2.374516	-1.199598	0.930735
C	-3.708156	-0.712528	1.275539
C	-4.621040	-1.716670	0.575089
C	-3.835913	-2.066346	-0.693065
C	-2.381448	-2.127229	-0.222986
C	-1.240515	-0.754197	1.430719
C	-1.003362	0.370102	2.194565
C	-0.265282	1.610295	0.376990
C	0.219606	0.430673	3.085166
N	0.495283	0.978253	-0.472695
C	4.538383	-0.052332	-0.014036
C	4.084340	1.188819	0.430479
C	2.762700	1.539606	0.282129
C	1.863556	0.647222	-0.294651
C	2.310077	-0.579879	-0.748387
C	3.647180	-0.929958	-0.609575
O	5.848852	-0.296927	0.172906
C	6.398132	-1.509523	-0.263298
C	-1.594003	2.146467	-0.137790
O	-1.488499	2.472292	-1.396782
O	-2.545322	2.331624	0.544515
C	-2.682925	2.824045	-2.083759
C	-1.332769	-1.639479	-1.250046
O	-1.492710	-0.463689	-1.639621
O	-0.413334	-2.403821	-1.498281
H	-3.860968	0.288798	0.898306
H	-3.829181	-0.695304	2.352528
H	-4.752342	-2.598383	1.195146
H	-5.601444	-1.302908	0.370128
H	-4.151687	-2.997864	-1.146574
H	-3.936770	-1.275562	-1.426265
H	-2.114639	-3.121695	0.114031
H	-0.383679	-1.337487	1.133383
H	-1.848015	0.955583	2.509391
H	0.192812	2.181947	1.157146
H	1.052588	-0.124945	2.666749
H	0.552219	1.454079	3.242949

```
      H         0.015617       0.019946       4.071303
      H        -0.015224       0.484864      -1.206926
      H         4.789820       1.867144       0.872159
      H         2.439428       2.515020       0.598896
      H         1.617577      -1.268051      -1.202992
      H         3.965083      -1.888792      -0.968746
      H         5.941830      -2.354371       0.241106
      H         6.290125      -1.629010      -1.335815
      H         7.447525      -1.470962      -0.013495
      H        -3.152444       3.673751      -1.611418
      H        -2.375861       3.066285      -3.087494
      H        -3.351018       1.976980      -2.090173
---------------------------------------------------------------------
 Statistical Thermodynamic Analysis
 Temperature= 298.150 Kelvin       Pressure= 1.00000 Atm
=====================================================================
 SCF Energy=     -1178.72758451         Predicted Change= -3.552982D-08
 Zero-point correction (ZPE)=      -1178.2896      0.43791
 Internal Energy (U)=                      -1178.2662      0.46135
 Enthalpy (H)=                             -1178.2652       0.46230
 Gibbs Free Energy (G)=                    -1178.3440       0.38350
---------------------------------------------------------------------
 Frequencies --  -385.7647               29.2599               33.2389

 Supporting Information: s-Trans-Si-3D-(Methyl-Syn)-(Esther-Anti).output
---------------------------------------------------------------------
 Using  Gaussian 03:  Al64T-G03RevC.01  3-Apr-2004
=====================================================================
 # opt=(calcfc,ts,maxcycle=150,noeigentest) freq=noraman hf/6-31g(d)
 geom=connectivity scf=(direct,tight,maxcycle=300)
 #N Geom=AllCheck Guess=Read SCRF=Check GenChk RHF/6-31G(d) Freq
---------------------------------------------------------------------
 Pointgroup= C1   Stoichiometry= C18H24N2O5   C1[X(C18H24N2O5)]  #Atoms= 49
 Charge = 0         Multiplicity = 1
---------------------------------------------------------------------
 SCF Energy= -1178.72819201   Predicted Change= -3.823938D-09
=====================================================================
 Optimization completed.            {Found        2        times}
 Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force      0.00000 ||  0.00045   [ YES ]      0.00000 ||  0.00030   [ YES ]
 Displ      0.00092 ||  0.00180   [ YES ]      0.00092 ||  0.00180   [ YES ]
---------------------------------------------------------------------
      Atomic             Coordinates (Angstroms)
       Type           X             Y         Z
---------------------------------------------------------------------
      N        -1.238687       1.514613       0.987649
      C         0.025475       1.719464       1.700296
      C         0.499742       3.097618       1.224135
      C        -0.788937       3.794038       0.776617
      C        -1.567791       2.654781       0.114666
      C        -2.075011       0.533543       1.237691
      C        -1.804473      -0.661137       1.875576
      C        -1.030797      -1.635952      -0.109801
      C        -2.922865      -1.518880       2.425075
      N        -0.117259      -0.887446      -0.636054
      C         4.028933      -1.033717       0.044165
      C         3.185230      -1.862937       0.778137
      C         1.822570      -1.828540       0.580914
      C         1.271248      -0.962392      -0.360329
      C         2.109047      -0.130696      -1.085837
      C         3.480723      -0.164798      -0.886979
      O         5.342563      -1.145470       0.311976
      C         6.264614      -0.353675      -0.385653
      C        -2.383463      -1.694844      -0.760648
      O        -2.927075      -2.873907      -0.542991
      O        -2.867356      -0.824590      -1.398512
      C        -4.202988      -3.110949      -1.128585
      C        -1.139257       2.495564      -1.376301
      O        -0.449818       1.497779      -1.678318
      O        -1.500934       3.416669      -2.076185
      H         0.741537       0.941336       1.481079
      H        -0.171811       1.705878       2.768343
      H         1.028851       3.630381       2.005378
      H         1.169579       2.983292       0.380582
      H        -1.332066       4.170375       1.639669
      H        -0.625988       4.609237       0.088044
      H        -2.636294       2.823104       0.132536
      H        -3.051540       0.665334       0.805011
      H        -0.851983      -0.758693       2.370378
      H        -0.754048      -2.503500       0.450379
      H        -3.852836      -1.351608       1.889893
      H        -2.693492      -2.578117       2.355277
      H        -3.112861      -1.303464       3.474001
      H        -0.404918      -0.031660      -1.160737
      H         3.618226      -2.527947       1.501440
      H         1.207213      -2.480245       1.172622
      H         1.681179       0.554667      -1.792607
      H         4.098779       0.492310      -1.466427
      H         6.228582      -0.551894      -1.451279
      H         6.091879       0.702356      -0.208955
      H         7.238591      -0.622819      -0.006495
      H        -4.925892      -2.406343      -0.745535
      H        -4.141366      -3.018041      -2.202199
      H        -4.468727      -4.116916      -0.848150
---------------------------------------------------------------------
 Statistical Thermodynamic Analysis
 Temperature= 298.150 Kelvin       Pressure= 1.00000 Atm
=====================================================================
 SCF Energy=     -1178.72819201         Predicted Change= -3.823938D-09
 Zero-point correction (ZPE)=      -1178.2911      0.43706
 Internal Energy (U)=                      -1178.2676      0.46055
 Enthalpy (H)=                             -1178.2666       0.46149
 Gibbs Free Energy (G)=                    -1178.3458       0.38232
---------------------------------------------------------------------
 Frequencies --  -335.0995               23.8204               31.9805
```

```
 Supporting Information: s-Trans-Si-3D-(Methyl-Syn)-(Esther-Syn).output
--------------------------------------------------------------------------------
 Using  Gaussian 03:  Al64T-G03RevC.01  3-Apr-2004
================================================================================
 #hf/6-31G* opt=(gdiis,calcfc,ts,noeigentest,maxcycle=300)
 scf=(maxcycle=300,direct) freq=noraman
 #N Geom=AllCheck Guess=Read SCRF=Check GenChk RHF/6-31G(d) Freq
--------------------------------------------------------------------------------
 Pointgroup= C1   Stoichiometry= C18H24N2O5   C1[X(C18H24N2O5)]  #Atoms= 49
 Charge = 0         Multiplicity = 1
--------------------------------------------------------------------------------
 SCF Energy= -1178.72983665   Predicted Change= -1.400913D-09
================================================================================
 Optimization completed.             {Found        2        times}
 Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force      0.00000 ||  0.00045   [ YES ]      0.00000 ||  0.00030   [ YES ]
 Displ      0.00076 ||  0.00180   [ YES ]      0.00076 ||  0.00180   [ YES ]
--------------------------------------------------------------------------------
      Atomic             Coordinates (Angstroms)
       Type           X             Y         Z
--------------------------------------------------------------------------------
       N        -1.272555       1.724564       0.944926
       C         0.022169       2.183868       1.443783
       C         0.343297       3.420498       0.587821
       C        -0.998779       3.825181      -0.034437
       C        -1.716285       2.496026      -0.226667
       C        -1.955208       0.704095       1.442950
       C        -1.465377      -0.288903       2.254240
       C        -1.085285      -1.670768       0.361385
       C        -2.348921      -1.123176       3.151531
       N        -0.186812      -1.161155      -0.420757
       C         3.971068      -0.882125       0.058785
       C         3.249934      -1.792864       0.828363
       C         1.885033      -1.901283       0.689256
       C         1.210205      -1.091965      -0.220143
       C         1.922415      -0.186305      -0.986952
       C         3.299119      -0.080484      -0.850667
       O         5.299322      -0.858025       0.269958
       C         6.106063       0.015434      -0.471780
       C        -2.480553      -1.861351      -0.223984
       O        -2.381036      -2.267528      -1.460296
       O        -3.486966      -1.746279       0.388300
       C        -3.572810      -2.265246      -2.241625
       C        -1.301630       1.693677      -1.487093
       O        -1.870195       0.581613      -1.577440
       O        -0.424424       2.149397      -2.200968
       H         0.785887       1.422174       1.344647
       H        -0.073203       2.422628       2.498527
       H         0.788919       4.209695       1.182017
       H         1.034704       3.156737      -0.199852
       H        -1.563980       4.450415       0.651630
       H        -0.875080       4.351230      -0.969146
       H        -2.796183       2.584260      -0.205581
       H        -2.978757       0.648225       1.121315
       H        -0.434672      -0.211848       2.561568
       H        -0.805107      -2.340072       1.147194
       H        -3.379855      -1.104649       2.828659
       H        -2.034521      -2.165440       3.178492
       H        -2.305166      -0.761232       4.176330
       H        -0.581577      -0.594667      -1.173298
       H         3.782447      -2.413099       1.524419
       H         1.361367      -2.627237       1.283597
       H         1.404851       0.451883      -1.682425
       H         3.820893       0.631738      -1.458751
       H         6.043235      -0.195222      -1.533764
       H         5.836332       1.050507      -0.292459
       H         7.117700      -0.151725      -0.135020
       H        -4.312533      -2.914576      -1.798426
       H        -3.941817      -1.254432      -2.311594
       H        -3.278615      -2.628440      -3.212283
--------------------------------------------------------------------------------
 Statistical Thermodynamic Analysis
 Temperature= 298.150 Kelvin       Pressure= 1.00000 Atm
================================================================================
 SCF Energy=     -1178.72983665         Predicted Change= -1.400913D-09
 Zero-point correction (ZPE)=      -1178.2919      0.43789
 Internal Energy (U)=                      -1178.2685      0.46129
 Enthalpy (H)=                             -1178.2675      0.46224
 Gibbs Free Energy (G)=                    -1178.3460      0.38376
--------------------------------------------------------------------------------
 Frequencies --  -311.6497               26.8917               34.1086

 Supporting Information: s-Trans-Si-3D-(Methyl-Syn)-(Esther-Syn)2.output
--------------------------------------------------------------------------------
 Using  Gaussian 03:  Al64T-G03RevC.01  3-Apr-2004
================================================================================
 # opt=(calcfc,ts,maxcycle=150,noeigentest) freq=noraman hf/6-31g(d)
 geom=connectivity scf=(direct,tight,maxcycle=300)
 #N Geom=AllCheck Guess=Read SCRF=Check GenChk RHF/6-31G(d) Freq
--------------------------------------------------------------------------------
 Pointgroup= C1   Stoichiometry= C18H24N2O5   C1[X(C18H24N2O5)]  #Atoms= 49
 Charge = 0         Multiplicity = 1
--------------------------------------------------------------------------------
 SCF Energy= -1178.73475146   Predicted Change= -5.162964D-08
================================================================================
 Optimization completed.             {Found        1        times}
 Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force      0.00002 ||  0.00045   [ YES ]      0.00000 ||  0.00030   [ YES ]
 Displ      0.00344 ||  0.00180   [ NO ]       0.00344 ||  0.00180   [ YES ]
--------------------------------------------------------------------------------
      Atomic             Coordinates (Angstroms)
       Type           X             Y         Z
--------------------------------------------------------------------------------
       N        -1.456171       1.108427       1.253720
       C        -0.178308       1.575374       1.795414
       C        -0.042847       3.004598       1.257239
```

C	-1.480670	3.424357	0.933546
C	-2.131728	2.130110	0.435488
C	-1.995933	-0.063050	1.507587
C	-1.373534	-1.198854	1.984665
C	-0.701816	-1.842178	-0.130289
C	-2.173393	-2.345430	2.560352
N	0.076268	-0.938987	-0.647236
C	4.220322	-0.470723	-0.134880
C	3.564732	-1.516789	0.508670
C	2.206099	-1.689443	0.363601
C	1.470127	-0.815808	-0.433101
C	2.119828	0.229314	-1.069167
C	3.487687	0.403075	-0.923606
O	5.547384	-0.391920	0.072209
C	6.289818	0.620635	-0.549612
C	-2.071525	-2.066982	-0.710075
O	-2.511762	-1.016035	-1.337023
O	-2.623300	-3.112337	-0.595864
C	-3.766088	-1.070093	-2.018152
C	-1.908481	1.914176	-1.087218
O	-0.769600	1.512529	-1.413837
O	-2.862415	2.184450	-1.791647
H	0.643635	0.948064	1.484678
H	-0.231618	1.549794	2.880161
H	0.434322	3.658375	1.978008
H	0.547799	2.997201	0.352863
H	-1.986763	3.767294	1.831663
H	-1.535281	4.213819	0.195466
H	-3.194884	2.104396	0.632465
H	-3.031178	-0.142010	1.220233
H	-0.363690	-1.098170	2.347315
H	-0.283280	-2.712730	0.327873
H	-3.171946	-2.388371	2.140234
H	-1.702321	-3.303243	2.360570
H	-2.272004	-2.257285	3.639656
H	-0.357812	-0.121587	-1.104345
H	4.140152	-2.186479	1.119601
H	1.739320	-2.509141	0.876925
H	1.549137	0.913784	-1.668203
H	3.957855	1.222029	-1.431385
H	6.225977	0.550340	-1.630001
H	5.960622	1.604037	-0.231787
H	7.314147	0.472893	-0.243508
H	-3.714802	-1.800656	-2.811726
H	-4.548363	-1.340488	-1.324000
H	-3.907914	-0.075195	-2.401627

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1178.73475146 Predicted Change= -5.162964D-08
Zero-point correction (ZPE)= -1178.2970 0.43774
Internal Energy (U)= -1178.2735 0.46117
Enthalpy (H)= -1178.2726 0.46212
Gibbs Free Energy (G)= -1178.3508 0.38387

Frequencies -- -343.5980 29.4364 32.0136

Supporting Information: s-Trans-Si-3D-(Methyl-Syn)-EW.output

Using Gaussian 03: Al64T-G03RevC.01 3-Apr-2004

==========

# hf/6-31g(d) geom=connectivity scf=(direct,maxcycle=300,tight)
opt=(maxcycle=250,ts,calcfc,noeigentest) freq=noraman
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RHF/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C18H24N2O5 C1[X(C18H24N2O5)] #Atoms= 49
Charge = 0 Multiplicity = 1

SCF Energy= -1178.72418360 Predicted Change= -7.036011D-08

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00004	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00362	0.00180	[NO]	0.00362	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
N	-1.219070	1.661855	0.989019
C	0.077003	2.005934	1.571014
C	0.500824	3.282128	0.825556
C	-0.791598	3.816411	0.195984
C	-1.581071	2.554678	-0.124218
C	-1.956189	0.619138	1.335023
C	-1.544505	-0.488220	2.035739
C	-1.070717	-1.667309	0.050740
C	-2.507994	-1.383110	2.779850
N	-0.128551	-1.089082	-0.627244
C	4.007428	-0.955209	0.066484
C	3.231963	-1.911821	0.717645
C	1.873146	-1.974821	0.506106
C	1.258872	-1.072001	-0.356544
C	2.025467	-0.120535	-1.006220
C	3.395955	-0.061166	-0.798348
O	5.324698	-0.981683	0.340110
C	6.184298	-0.073221	-0.291641
C	-2.371981	-1.886811	-0.710212
O	-3.465550	-1.485916	-0.124467
O	-2.316821	-2.482099	-1.731284
C	-4.663930	-1.610498	-0.886945
C	-1.177463	1.825661	-1.433059
O	-1.806433	0.761422	-1.622096
O	-0.248773	2.279735	-2.081324
H	0.800938	1.211167	1.442543
H	-0.049995	2.171122	2.636545

H	0.971811	3.994116	1.493156
H	1.202534	3.036404	0.041260
H	-1.341951	4.421759	0.911443
H	-0.603068	4.403820	-0.690062
H	-2.653902	2.708937	-0.121680
H	-2.963418	0.647911	0.967150
H	-0.532255	-0.491583	2.406913
H	-0.823424	-2.418065	0.771946
H	-3.525530	-1.249443	2.437998
H	-2.261454	-2.438317	2.665808
H	-2.485331	-1.175820	3.846973
H	-0.476671	-0.454842	-1.343719
H	3.717647	-2.604730	1.378544
H	1.308631	-2.739729	1.006676
H	1.553732	0.587124	-1.665860
H	3.960727	0.687737	-1.317508
H	6.164141	-0.194614	-1.369144
H	5.931732	0.950927	-0.039123
H	7.175663	-0.294805	0.072991
H	-4.573986	-1.029602	-1.791495
H	-4.850342	-2.646496	-1.125352
H	-5.446894	-1.219418	-0.257643

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1178.72418360 Predicted Change= -7.036011D-08
Zero-point correction (ZPE)= -1178.2863 0.43782
Internal Energy (U)= -1178.2628 0.46132
Enthalpy (H)= -1178.2619 0.46227
Gibbs Free Energy (G)= -1178.3409 0.38321

Frequencies -- -321.1312 27.3948 33.6774

Supporting Information: s-Trans-Si-3U-(Methyl-Anti)-(Esther-Anti).output

---

Using Gaussian 03: Al64T-G03RevC.01 3-Apr-2004

==========

# opt=(calcfc,ts,maxcycle=150,noeigentest) freq=noraman hf/6-31g(d)
geom=connectivity scf=(direct,tight,maxcycle=300)
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RHF/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C18H24N2O5 C1[X(C18H24N2O5)] #Atoms= 49
Charge = 0 Multiplicity = 1

SCF Energy= -1178.72476431 Predicted Change= -5.196492D-08

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00003	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00491	0.00180	[NO]	0.00491	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
N	-1.053632	1.566540	0.993135
C	0.191019	1.792266	1.726930
C	0.337277	3.311427	1.685811
C	-0.217988	3.667279	0.306670
C	-1.389930	2.693960	0.095542
C	-1.915106	0.609366	1.264036
C	-1.675439	-0.576538	1.928591
C	-0.971879	-1.618512	-0.041991
C	-2.815712	-1.387444	2.504750
N	-0.158353	-0.849454	-0.689622
C	4.029362	-0.669717	-0.371895
C	3.327557	-1.521582	0.462536
C	1.940572	-1.590196	0.379854
C	1.249331	-0.816844	-0.531812
C	1.959672	0.048274	-1.368403
C	3.329001	0.117201	-1.286426
O	5.367465	-0.526699	-0.374437
C	6.151474	-1.289314	0.498865
C	-2.366129	-1.819493	-0.569102
O	-2.748301	-3.055814	-0.321547
O	-3.005983	-1.007174	-1.140363
C	-4.036835	-3.435034	-0.794253
C	-1.523412	2.357167	-1.414847
O	-0.853704	1.388557	-1.840996
O	-2.207084	3.145502	-2.028291
H	1.024017	1.305504	1.234750
H	0.107099	1.397152	2.731028
H	-0.266780	3.759676	2.469096
H	1.363684	3.628689	1.828885
H	-0.539169	4.695893	0.219001
H	0.538063	3.488567	-0.450243
H	-2.321461	3.134512	0.427998
H	-2.884937	0.752723	0.818938
H	-0.722606	-0.693479	2.418752
H	-0.587877	-2.427316	0.542567
H	-3.739195	-1.216000	1.959804
H	-2.609540	-2.453264	2.476858
H	-3.004318	-1.128018	3.543887
H	-0.552745	-0.045208	-1.235148
H	3.830946	-2.137976	1.181173
H	1.431955	-2.260262	1.047605
H	1.418676	0.665111	-2.060887
H	3.883238	0.777794	-1.926175
H	5.913118	-1.074141	1.535299
H	6.030197	-2.351474	0.314096
H	7.175930	-1.010148	0.305641
H	-4.084872	-3.326423	-1.867065
H	-4.157979	-4.467525	-0.510265
H	-4.797703	-2.822571	-0.334231

Statistical Thermodynamic Analysis

```
 Temperature= 298.150 Kelvin       Pressure= 1.00000 Atm
 ============================================================================
 SCF Energy=     -1178.72476431         Predicted Change= -5.196492D-08
 Zero-point correction (ZPE)=      -1178.2880      0.43669
 Internal Energy (U)=                      -1178.2644      0.46030
 Enthalpy (H)=                             -1178.2635      0.46124
 Gibbs Free Energy (G)=                    -1178.3434      0.38133
 ----------------------------------------------------------------------------
 Frequencies --  -341.8275               21.7791               32.6269

 Supporting Information: s-Trans-Si-3U-(Methyl-Anti)-(Esther-Syn).output
 ----------------------------------------------------------------------------
 Using  Gaussian 03:  Al64T-G03RevC.01  3-Apr-2004
 ============================================================================
 # hf/6-31g(d) geom=connectivity scf=(direct,maxcycle=300,tight)
 opt=(maxcycle=250,ts,calcfc,noeigentest) freq=noraman
 #N Geom=AllCheck Guess=Read SCRF=Check GenChk RHF/6-31G(d) Freq
 ----------------------------------------------------------------------------
 Pointgroup= C1   Stoichiometry= C18H24N2O5   C1[X(C18H24N2O5)]  #Atoms= 49
 Charge = 0         Multiplicity = 1
 ----------------------------------------------------------------------------
 SCF Energy= -1178.73333904   Predicted Change= -1.065985D-07
 ============================================================================
 Optimization completed.            {Found        1        times}
 Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force      0.00003 ||  0.00045   [ YES ]      0.00000 ||  0.00030   [ YES ]
 Displ      0.00771 ||  0.00180   [ NO ]       0.00771 ||  0.00180   [ NO ]
 ----------------------------------------------------------------------------
      Atomic             Coordinates (Angstroms)
       Type           X             Y         Z
 ----------------------------------------------------------------------------
       N        -1.240376       1.354868       1.113335
       C         0.025418       1.812392       1.681849
       C        -0.048812       3.325820       1.493408
       C        -0.801699       3.470346       0.168338
       C        -1.842079       2.345479       0.188597
       C        -1.876205       0.257247       1.466897
       C        -1.348782      -0.857038       2.086961
       C        -0.687569      -1.809885       0.076958
       C        -2.238995      -1.861855       2.783575
       N         0.009694      -0.969645      -0.628107
       C         4.141980      -0.221357      -0.468988
       C         3.607605      -1.224368       0.320595
       C         2.241703      -1.484153       0.287356
       C         1.404662      -0.747835      -0.527562
       C         1.945014       0.267127      -1.320880
       C         3.294428       0.522743      -1.289558
       O         5.445400       0.110129      -0.512623
       C         6.371371      -0.600187       0.260584
       C        -2.062555      -2.211909      -0.382601
       O        -2.614051      -1.290752      -1.109712
       O        -2.515385      -3.272826      -0.098546
       C        -3.901533      -1.505741      -1.687244
       C        -2.102563       1.707451      -1.204796
       O        -1.086166       1.244595      -1.766532
       O        -3.260560       1.706004      -1.579017
       H         0.867976       1.392899       1.146606
       H         0.094021       1.511964       2.720045
       H        -0.615340       3.770310       2.306127
       H         0.932953       3.784381       1.478466
       H        -1.267101       4.440806       0.049192
       H        -0.128193       3.310346      -0.663513
       H        -2.784693       2.680436       0.603959
       H        -2.901845       0.222877       1.139141
       H        -0.338763      -0.786198       2.457776
       H        -0.194537      -2.558200       0.659493
       H        -3.240243      -1.866344       2.367067
       H        -1.852891      -2.872416       2.697082
       H        -2.326746      -1.639963       3.844489
       H        -0.498358      -0.274388      -1.196674
       H         4.227674      -1.817378       0.963658
       H         1.866791      -2.275616       0.908888
       H         1.289988       0.850074      -1.940810
       H         3.719044       1.299776      -1.896845
       H         6.160006      -0.502213       1.320271
       H         6.387500      -1.651026      -0.008375
       H         7.336215      -0.164931       0.049983
       H        -4.614304      -1.746475      -0.912182
       H        -4.139847      -0.570986      -2.161868
       H        -3.846783      -2.317153      -2.398064
 ----------------------------------------------------------------------------
 Statistical Thermodynamic Analysis
 Temperature= 298.150 Kelvin       Pressure= 1.00000 Atm
 ============================================================================
 SCF Energy=     -1178.73333904         Predicted Change= -1.065985D-07
 Zero-point correction (ZPE)=      -1178.2956      0.43767
 Internal Energy (U)=                      -1178.2722      0.46113
 Enthalpy (H)=                             -1178.2712      0.46208
 Gibbs Free Energy (G)=                    -1178.3499      0.38336
 ----------------------------------------------------------------------------
 Frequencies --  -334.0180               22.0279               31.1287

 Supporting Information: s-Trans-Si-3U-(Methyl-Anti)-EW.output
 ----------------------------------------------------------------------------
 Using  Gaussian 03:  Al64T-G03RevC.01  3-Apr-2004
 ============================================================================
 #hf/6-31G* opt=(gdiis,ts,noeigentest,calcfc,maxcycle=300)
 scf=(maxcycle=300) freq=noraman
 #N Geom=AllCheck Guess=Read SCRF=Check GenChk RHF/6-31G(d) Freq
 ----------------------------------------------------------------------------
 Pointgroup= C1   Stoichiometry= C18H24N2O5   C1[X(C18H24N2O5)]  #Atoms= 49
 Charge = 0         Multiplicity = 1
 ----------------------------------------------------------------------------
 SCF Energy= -1178.72709534   Predicted Change= -8.164340D-11
 ============================================================================
 Optimization completed.            {Found        2        times}
```

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00024	0.00180	[YES]	0.00024	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
N	-1.273567	1.511027	0.982120
C	-0.032406	2.220329	1.274101
C	-0.300009	3.623350	0.728732
C	-1.216815	3.358096	-0.466186
C	-2.122864	2.215087	0.010208
C	-1.706101	0.443141	1.646196
C	-0.953874	-0.428034	2.383847
C	-0.616911	-1.709468	0.371751
C	-1.555920	-1.392088	3.377517
N	0.063898	-0.981025	-0.447805
C	4.177009	-0.154030	-0.553139
C	3.669913	-0.921570	0.481298
C	2.309339	-1.202262	0.540418
C	1.451450	-0.725813	-0.430430
C	1.965103	0.049753	-1.469978
C	3.307706	0.332117	-1.530008
O	5.471585	0.176343	-0.702053
C	6.419333	-0.277406	0.224396
C	-2.030853	-2.114219	-0.040101
O	-2.001092	-2.554135	-1.266988
O	-2.963756	-2.127271	0.687307
C	-3.256237	-2.710450	-1.931886
C	-2.623163	1.363648	-1.181179
O	-2.006755	0.296427	-1.423074
O	-3.556625	1.846205	-1.783237
H	0.815826	1.763997	0.775062
H	0.162587	2.207707	2.340282
H	-0.818288	4.216526	1.476056
H	0.613638	4.142743	0.463329
H	-1.792143	4.218727	-0.777302
H	-0.628791	3.027004	-1.317363
H	-2.995423	2.615991	0.514837
H	-2.752062	0.230520	1.518250
H	0.089735	-0.194013	2.523991
H	-0.120253	-2.366996	1.055543
H	-2.605959	-1.558989	3.181804
H	-1.061372	-2.361804	3.353152
H	-1.453498	-1.018261	4.393903
H	-0.533274	-0.402402	-1.056416
H	4.308139	-1.308097	1.251202
H	1.948732	-1.793624	1.361016
H	1.301067	0.422333	-2.229237
H	3.710725	0.926078	-2.328309
H	6.210719	0.100026	1.219781
H	6.459358	-1.361099	0.249387
H	7.371667	0.105794	-0.108117
H	-3.711349	-1.738181	-2.032914
H	-3.015956	-3.120719	-2.898836
H	-3.891208	-3.384902	-1.378294

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

SCF Energy=	-1178.72709534	Predicted Change= -8.164340D-11
Zero-point correction (ZPE)=	-1178.2901	0.43691
Internal Energy (U)=	-1178.2665	0.46053
Enthalpy (H)=	-1178.2656	0.46147
Gibbs Free Energy (G)=	-1178.3452	0.38182

Frequencies -- -276.6720 18.4877 32.1715

Supporting Information: s-Cis-Re-3D-(Methyl-Syn)-(Esther-Syn).output

Using Gaussian 03: Al64T-G03RevC.01 3-Apr-2004

```
#hf/6-31g* scf=(direct,tight,maxcycle=300)
opt=(calcfc,maxcycle=150,ts,noeigentest) freq=noraman
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RHF/6-31G(d) Freq
```

Pointgroup= C1 Stoichiometry= C18H24N2O5 C1[X(C18H24N2O5)] #Atoms= 49
Charge = 0 Multiplicity = 1

SCF Energy= -1178.72895441 Predicted Change= -2.836096D-09

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00001	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00120	0.00180	[YES]	0.00120	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
N	2.714871	0.883153	0.825957
C	4.033226	1.002841	0.199134
C	4.010507	2.388185	-0.454022
C	2.964928	3.153133	0.362591
C	1.901163	2.084866	0.637226
C	2.322905	-0.221808	1.423506
C	1.069496	-0.575945	1.885179
C	0.176022	-1.778746	0.077240
C	0.957407	-1.610367	2.988490
N	-0.514991	-0.989911	-0.683005
C	-4.544687	-0.006426	-0.015932
C	-3.641304	0.966380	-0.412756
C	-2.308934	0.640853	-0.629637
C	-1.879650	-0.660448	-0.445845
C	-2.791353	-1.645221	-0.073450
C	-4.108782	-1.320248	0.149838
O	-5.850882	0.210760	0.222075

C	-6.380158	1.499206	0.069046
C	0.901244	1.979928	-0.538136
O	0.026304	2.833120	-0.534737
O	1.093885	1.056031	-1.349762
C	1.458368	-2.405897	-0.396099
O	1.895597	-1.893608	-1.511458
O	1.950470	-3.314760	0.192017
C	3.072393	-2.450053	-2.080015
H	4.185257	0.213553	-0.525705
H	4.807679	0.927866	0.957659
H	4.988052	2.855653	-0.444828
H	3.681402	2.300437	-1.481294
H	3.394721	3.501851	1.297460
H	2.545952	4.002623	-0.158204
H	1.343599	2.292610	1.540619
H	3.108473	-0.952756	1.544788
H	-0.041514	-2.034262	3.035517
H	1.653789	-2.428989	2.838208
H	1.155396	-1.181165	3.968125
H	0.018784	-0.349638	-1.278659
H	-3.944165	1.985144	-0.552411
H	-1.616573	1.412183	-0.916507
H	-2.481534	-2.671030	0.018560
H	-4.822988	-2.069623	0.434677
H	-5.907377	2.203238	0.744894
H	-6.273003	1.851453	-0.950992
H	-7.429367	1.423062	0.310994
H	-0.329125	-2.349850	0.826742
H	0.293086	0.169935	1.849799
H	3.270082	-1.862722	-2.960751
H	3.894625	-2.380733	-1.383454
H	2.905863	-3.485284	-2.339135

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

SCF Energy= -1178.72895441 Predicted Change= -2.836096D-09
Zero-point correction (ZPE)= -1178.2915 0.43737
Internal Energy (U)= -1178.2679 0.46102
Enthalpy (H)= -1178.2669 0.46196
Gibbs Free Energy (G)= -1178.3466 0.38234

Frequencies -- -343.3812 26.7189 28.3309

Supporting Information: s-Cis-Re-3U-(Methyl-Syn)-(Esther-Syn).output

---

Using Gaussian 03: Al64T-G03RevC.01 3-Apr-2004

# opt=(calcfc,ts,maxcycle=150,noeigentest) freq=noraman hf/6-31g(d)
geom=connectivity scf=(direct,tight,maxcycle=300)
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RHF/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C18H24N2O5 C1[X(C18H24N2O5)] #Atoms= 49

Charge = 0 Multiplicity = 1

SCF Energy= -1178.73093062 Predicted Change= -1.241419D-07

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00002	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00674	0.00180	[NO]	0.00674	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
N	-2.862789	-1.000658	0.819330
C	-4.295994	-0.742111	0.742320
C	-4.816827	-1.972870	0.010347
C	-3.695560	-2.261022	-0.992460
C	-2.398956	-1.899483	-0.244519
C	-2.079701	-0.417537	1.709531
C	-0.706589	-0.435770	1.791984
C	-0.114845	1.434711	0.476094
C	-0.041121	-0.083359	3.107035
N	0.657270	0.988461	-0.464449
C	4.674845	-0.132327	-0.002119
C	3.785546	-0.965788	-0.662432
C	2.455524	-0.593552	-0.806474
C	2.017946	0.612947	-0.295338
C	2.913395	1.461720	0.347785
C	4.228218	1.087907	0.503073
O	5.978191	-0.403666	0.194136
C	6.520538	-1.600768	-0.290870
C	-1.369513	-1.230237	-1.175272
O	-1.628042	-0.058241	-1.510246
O	-0.389980	-1.900115	-1.476076
C	-1.422811	2.110606	0.090570
O	-1.295923	2.709362	-1.063188
O	-2.356897	2.199124	0.814782
C	-2.480924	3.225771	-1.654617
H	-4.484139	0.162921	0.174682
H	-4.713502	-0.617984	1.734426
H	-4.928341	-2.797368	0.708136
H	-5.775932	-1.799798	-0.463766
H	-3.684198	-3.286546	-1.338836
H	-3.800770	-1.614021	-1.855222
H	-1.943438	-2.772753	0.206547
H	-2.613331	0.164700	2.439191
H	0.975970	0.269912	2.960266
H	-0.587882	0.695957	3.632643
H	0.026328	-0.939125	3.775213
H	0.159835	0.663710	-1.286288
H	4.100866	-1.908458	-1.064174
H	1.752640	-1.242650	-1.296957
H	2.589590	2.422388	0.707101
H	4.933062	1.731674	0.994528

```
      H         6.042768      -2.462982       0.161438
      H         6.433658      -1.665256      -1.370004
      H         7.564881      -1.589285      -0.018229
      H         0.328095       1.770882       1.390413
      H        -0.169016      -1.114958       1.154224
      H        -2.168268       3.671439      -2.584655
      H        -3.165843       2.412462      -1.837167
      H        -2.932211       3.965759      -1.010794
---------------------------------------------------------------------------
 Statistical Thermodynamic Analysis
 Temperature= 298.150 Kelvin       Pressure= 1.00000 Atm
===========================================================================
 SCF Energy=     -1178.73093062         Predicted Change= -1.241419D-07
 Zero-point correction (ZPE)=      -1178.2929      0.43801
 Internal Energy (U)=                      -1178.2695      0.46140
 Enthalpy (H)=                            -1178.2685       0.46234
 Gibbs Free Energy (G)=                   -1178.3467       0.38416
---------------------------------------------------------------------------
 Frequencies --  -358.0984               32.3287               36.4093

 Supporting Information: s-Cis-Si-3D-(Methyl-Anti)-(Esther-Anti).output
---------------------------------------------------------------------------
 Using  Gaussian 03:  IA32L-G03RevC.02 12-Jun-2004
===========================================================================
 # opt=(calcfc,ts,maxcycle=150,noeigentest) freq=noraman hf/6-31g(d)
 geom=connectivity scf=(direct,tight,maxcycle=300)
 #N Geom=AllCheck Guess=Read SCRF=Check GenChk RHF/6-31G(d) Freq
---------------------------------------------------------------------------
 Pointgroup= C1   Stoichiometry= C18H24N2O5   C1[X(C18H24N2O5)]  #Atoms= 49
 Charge = 0         Multiplicity = 1
---------------------------------------------------------------------------
 SCF Energy= -1178.72183168   Predicted Change= -2.098532D-09
===========================================================================
 Optimization completed.            {Found        2        times}
 Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force      0.00000 ||  0.00045   [ YES ]      0.00000 ||  0.00030   [ YES ]
 Displ      0.00132 ||  0.00180   [ YES ]      0.00132 ||  0.00180   [ YES ]
---------------------------------------------------------------------------
      Atomic             Coordinates (Angstroms)
       Type           X             Y         Z
---------------------------------------------------------------------------
       N        -0.827746       1.464654       1.096756
       C         0.280846       2.420756       1.222439
       C        -0.299737       3.752485       0.721824
       C        -1.816300       3.538802       0.774861
       C        -1.954117       2.068442       0.366995
       C        -0.829885       0.334977       1.769494
       C        -1.746943      -0.694201       1.753878
       C        -0.815872      -1.716303      -0.188721
       C        -1.702172      -1.763470       2.823571
       N        -0.048086      -0.912157      -0.843256
       C         4.094683      -0.372352      -0.406395
       C         3.352905       0.368559      -1.327426
       C         1.997534       0.183733      -1.447687
       C         1.343665      -0.755571      -0.645055
       C         2.075332      -1.483520       0.272967
       C         3.448356      -1.296707       0.395317
       O         5.414296      -0.114779      -0.370564
       C         6.239909      -0.823430       0.510349
       C        -1.883412       1.953570      -1.189348
       O        -2.838660       2.441810      -1.750126
       O        -0.850875       1.436193      -1.672974
       C        -2.213924      -1.937349      -0.690568
       O        -2.716638      -3.037115      -0.166047
       O        -2.755541      -1.239732      -1.473939
       C        -4.039853      -3.382943      -0.561899
       H         1.127362       2.095895       0.633255
       H         0.585748       2.479375       2.262122
       H         0.035468       4.587499       1.325619
       H         0.012137       3.929468      -0.299464
       H        -2.185054       3.683192       1.787134
       H        -2.367275       4.183591       0.107312
       H        -2.884916       1.635864       0.703630
       H         0.061529       0.185170       2.358329
       H        -2.027980      -2.725411       2.440610
       H        -0.695828      -1.888662       3.215622
       H        -2.347837      -1.524719       3.665961
       H        -0.495132      -0.125890      -1.362749
       H         3.864584       1.086741      -1.939907
       H         1.423550       0.769260      -2.140243
       H         1.610029      -2.210977       0.911566
       H         3.985065      -1.881184       1.116460
       H         5.958326      -0.648791       1.543496
       H         6.215458      -1.888321       0.304746
       H         7.240641      -0.453357       0.348374
       H        -0.399826      -2.495214       0.413435
       H        -2.712394      -0.493349       1.322589
       H        -4.270606      -4.295805      -0.037502
       H        -4.728697      -2.599397      -0.283647
       H        -4.080267      -3.536348      -1.629633
---------------------------------------------------------------------------
 Statistical Thermodynamic Analysis
 Temperature= 298.150 Kelvin       Pressure= 1.00000 Atm
===========================================================================
 SCF Energy=     -1178.72183168         Predicted Change= -2.098532D-09
 Zero-point correction (ZPE)=      -1178.2851      0.43667
 Internal Energy (U)=                      -1178.2615      0.46032
 Enthalpy (H)=                            -1178.2605       0.46126
 Gibbs Free Energy (G)=                   -1178.3402       0.38155
---------------------------------------------------------------------------
 Frequencies --  -321.3832               26.6393               29.8186

 Supporting Information: s-Cis-Si-3D-(Methyl-Anti)-(Esther-Syn).output
---------------------------------------------------------------------------
 Using  Gaussian 03:  IA32L-G03RevC.02 12-Jun-2004
===========================================================================
```

```
 # opt=(calcfc,ts,maxcycle=150,noeigentest) freq=noraman hf/6-31g(d)
 geom=connectivity scf=(direct,tight,maxcycle=300)
 #N Geom=AllCheck Guess=Read SCRF=Check GenChk RHF/6-31G(d) Freq
--------------------------------------------------------------------------------
 Pointgroup= C1   Stoichiometry= C18H24N2O5   C1[X(C18H24N2O5)]  #Atoms= 49
 Charge = 0         Multiplicity = 1
--------------------------------------------------------------------------------
 SCF Energy= -1178.73150774   Predicted Change= -7.686978D-08
================================================================================
 Optimization completed.            {Found        1        times}
 Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force      0.00001 ||  0.00045   [ YES ]      0.00000 ||  0.00030   [ YES ]
 Displ      0.01922 ||  0.00180   [ NO ]       0.01922 ||  0.00180   [ NO ]
--------------------------------------------------------------------------------
      Atomic             Coordinates (Angstroms)
       Type           X             Y         Z
--------------------------------------------------------------------------------
       N        -0.937990       1.412953       1.173257
       C         0.069980       2.479889       1.192878
       C        -0.589875       3.636126       0.435523
       C        -2.087360       3.353071       0.582215
       C        -2.159688       1.824810       0.466739
       C        -0.780352       0.307344       1.871587
       C        -1.589481      -0.805865       1.925397
       C        -0.610584      -1.878224       0.056773
       C        -1.412644      -1.833170       3.021815
       N         0.055247      -1.072407      -0.708472
       C         4.128594      -0.064399      -0.483715
       C         3.239360       0.661768      -1.275839
       C         1.908746       0.323066      -1.328819
       C         1.430610      -0.759305      -0.586279
       C         2.311083      -1.483170       0.194132
       C         3.656577      -1.137845       0.252046
       O         5.407591       0.351194      -0.501196
       C         6.374892      -0.336090       0.242272
       C        -2.228622       1.411884      -1.031214
       O        -3.352761       1.435635      -1.497048
       O        -1.142121       1.156174      -1.591582
       C        -1.985736      -2.343076      -0.339082
       O        -2.547356      -1.525696      -1.172970
       O        -2.428691      -3.361539       0.083955
       C        -3.876125      -1.775278      -1.630859
       H         0.987085       2.147312       0.725403
       H         0.287687       2.751121       2.221894
       H        -0.295615       4.598665       0.836969
       H        -0.309779       3.598693      -0.608380
       H        -2.438706       3.668832       1.560844
       H        -2.694829       3.836357      -0.170142
       H        -3.025495       1.424734       0.974120
       H         0.148529       0.270477       2.419382
       H        -1.691106      -2.824764       2.680055
       H        -0.381474      -1.874062       3.364625
       H        -2.032336      -1.612551       3.887877
       H        -0.488594      -0.398140      -1.267713
       H         3.616793       1.491268      -1.843605
       H         1.220815       0.892857      -1.924354
       H         1.987274      -2.335759       0.761276
       H         4.311699      -1.723513       0.866399
       H         6.153396      -0.305242       1.303915
       H         6.459991      -1.368697      -0.078924
       H         7.310133       0.170708       0.060393
       H        -0.097087      -2.545194       0.714753
       H        -2.581741      -0.715798       1.518162
       H        -4.153175      -0.878540      -2.154786
       H        -3.877315      -2.640372      -2.277849
       H        -4.526480      -1.947571      -0.786512
--------------------------------------------------------------------------------
 Statistical Thermodynamic Analysis
 Temperature= 298.150 Kelvin       Pressure= 1.00000 Atm
================================================================================
 SCF Energy=     -1178.73150774         Predicted Change= -7.686978D-08
 Zero-point correction (ZPE)=      -1178.2940      0.43745
 Internal Energy (U)=                        -1178.2705      0.46099
 Enthalpy (H)=                               -1178.2695      0.46194
 Gibbs Free Energy (G)=                      -1178.3491      0.38240
--------------------------------------------------------------------------------
 Frequencies --  -322.0500               10.6624               32.0141

 Supporting Information: s-Cis-Si-3D-(Methyl-Syn)-(Esther-Anti).output
--------------------------------------------------------------------------------
 Using  Gaussian 03:  Al64T-G03RevC.01  3-Apr-2004
================================================================================
 # hf/6-31g(d) geom=connectivity scf=(direct,maxcycle=300,tight)
 opt=(maxcycle=250,ts,calcfc,noeigentest) freq=noraman
 #N Geom=AllCheck Guess=Read SCRF=Check GenChk RHF/6-31G(d) Freq
--------------------------------------------------------------------------------
 Pointgroup= C1   Stoichiometry= C18H24N2O5   C1[X(C18H24N2O5)]  #Atoms= 49
 Charge = 0         Multiplicity = 1
--------------------------------------------------------------------------------
 SCF Energy= -1178.72252053   Predicted Change= -1.336334D-08
================================================================================
 Optimization completed.            {Found        1        times}
 Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force      0.00001 ||  0.00045   [ YES ]      0.00000 ||  0.00030   [ YES ]
 Displ      0.00287 ||  0.00180   [ NO ]       0.00287 ||  0.00180   [ YES ]
--------------------------------------------------------------------------------
      Atomic             Coordinates (Angstroms)
       Type           X             Y         Z
--------------------------------------------------------------------------------
       N        -0.760318       1.505950       1.089275
       C         0.431348       2.342236       1.283959
       C         0.030892       3.719469       0.731431
       C        -1.499408       3.663405       0.666819
       C        -1.756956       2.207647       0.265140
       C        -0.929615       0.394466       1.769865
       C        -1.946411      -0.534353       1.696102
```

C	-0.989220	-1.691767	-0.146907
C	-2.094401	-1.578725	2.781246
N	-0.091419	-0.993992	-0.758063
C	4.044604	-0.892593	-0.026824
C	3.461317	-0.078173	-0.986247
C	2.092453	-0.124545	-1.199920
C	1.291958	-0.983061	-0.462897
C	1.878796	-1.796171	0.503735
C	3.238758	-1.749490	0.717569
O	5.358750	-0.924724	0.258263
C	6.246550	-0.109044	-0.456181
C	-1.573819	2.055129	-1.278918
O	-2.423080	2.630451	-1.922010
O	-0.567092	1.421872	-1.669263
C	-2.360479	-1.774781	-0.753407
O	-3.019399	-2.799978	-0.251706
O	-2.760718	-1.043174	-1.589273
C	-4.338323	-3.011041	-0.744615
H	1.276609	1.920184	0.757812
H	0.669118	2.384877	2.341657
H	0.402567	4.524402	1.354477
H	0.437048	3.849549	-0.263472
H	-1.928433	3.863922	1.645154
H	-1.926916	4.348694	-0.049113
H	-2.751324	1.879382	0.530172
H	-0.104136	0.162779	2.424735
H	-2.495639	-2.507787	2.388996
H	-1.137967	-1.803437	3.246788
H	-2.767853	-1.253267	3.571197
H	-0.411589	-0.180054	-1.322118
H	4.050010	0.597205	-1.575212
H	1.636749	0.521299	-1.926009
H	1.294391	-2.474158	1.097230
H	3.699370	-2.374604	1.459174
H	6.230460	-0.341194	-1.515401
H	6.019603	0.941885	-0.313406
H	7.229107	-0.317119	-0.061180
H	-0.706590	-2.495224	0.498603
H	-2.851288	-0.240909	1.192499
H	-4.707050	-3.880019	-0.224559
H	-4.956491	-2.150949	-0.534860
H	-4.313554	-3.186401	-1.809445

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1178.72252053 Predicted Change= -1.336334D-08
Zero-point correction (ZPE)= -1178.2857 0.43678
Internal Energy (U)= -1178.2620 0.46044
Enthalpy (H)= -1178.2611 0.46139
Gibbs Free Energy (G)= -1178.3409 0.38161

Frequencies -- -323.4870 27.5171 28.9670

Supporting Information: s-Cis-Si-3D-(Methyl-Syn)-(Esther-Anti)2.output

---

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

# opt=(calcfc,ts,maxcycle=150,noeigentest) freq=noraman hf/6-31g(d)
geom=check guess=read scf=(direct,tight,maxcycle=300)
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RHF/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C18H24N2O5 C1[X(C18H24N2O5)] #Atoms= 49
Charge = 0 Multiplicity = 1

SCF Energy= -1178.71969856 Predicted Change= -5.136462D-09

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00004	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00103	0.00180	[YES]	0.00103	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
N	-0.415185	1.761291	0.873615
C	0.848190	2.366391	1.311578
C	0.723406	3.853669	0.921575
C	-0.582184	3.952254	0.105978
C	-0.906629	2.512997	-0.297585
C	-1.066485	0.889708	1.613629
C	-2.281344	0.268212	1.404787
C	-1.511528	-1.473371	-0.007249
C	-2.961769	-0.400221	2.583307
N	-0.485318	-1.112265	-0.702653
C	3.582505	-1.592960	0.238575
C	3.180964	-0.815300	-0.836602
C	1.833364	-0.666358	-1.125774
C	0.874722	-1.288821	-0.342182
C	1.278735	-2.073348	0.735408
C	2.617448	-2.220888	1.021854
O	4.861124	-1.799561	0.602674
C	5.896966	-1.209536	-0.134643
C	-0.113989	2.032341	-1.551020
O	0.957716	2.579954	-1.751184
O	-0.631146	1.088764	-2.177801
C	-2.853078	-1.490763	-0.686929
O	-3.685490	-2.269390	-0.024164
O	-3.098865	-0.928255	-1.695308
C	-4.994126	-2.410189	-0.565081
H	1.671482	1.896484	0.793129
H	0.972007	2.213100	2.376075
H	0.686207	4.483993	1.803192
H	1.570501	4.150007	0.323330
H	-1.385765	4.342053	0.724300
H	-0.474505	4.590801	-0.758851

```
      H        -1.960280       2.327396      -0.436954
      H        -0.523072       0.600348       2.498767
      H        -3.564582      -1.247420       2.277941
      H        -2.232447      -0.762256       3.303623
      H        -3.621486       0.284857       3.111931
      H        -0.653017      -0.432061      -1.464387
      H         3.893238      -0.310358      -1.458370
      H         1.530382      -0.043951      -1.946438
      H         0.567077      -2.585621       1.355767
      H         2.938578      -2.825961       1.848752
      H         5.893501      -1.551971      -1.163599
      H         5.829335      -0.127434      -0.114607
      H         6.816066      -1.517828       0.339925
      H        -1.398280      -2.127543       0.829604
      H        -2.924886       0.682492       0.647822
      H        -5.513973      -3.078573       0.101683
      H        -5.487597      -1.450431      -0.601853
      H        -4.942665      -2.828298      -1.559011
 ---------------------------------------------------------------------------
 Statistical Thermodynamic Analysis
 Temperature= 298.150 Kelvin       Pressure= 1.00000 Atm
 ===========================================================================
 SCF Energy=     -1178.71969856         Predicted Change= -5.136462D-09
 Zero-point correction (ZPE)=      -1178.2823      0.43730
 Internal Energy (U)=                      -1178.2587      0.46099
 Enthalpy (H)=                             -1178.2577      0.46193
 Gibbs Free Energy (G)=                    -1178.3378      0.38186
 ---------------------------------------------------------------------------
 Frequencies --  -339.4115               22.9344               27.9273

 Supporting Information: s-Cis-Si-3D-(Methyl-Syn)-(Esther-Syn).output
 ---------------------------------------------------------------------------
 Using  Gaussian 03:  Al64T-G03RevC.01  3-Apr-2004
 ===========================================================================
 #hf/6-31G* scf=(direct,tight,maxcycle=300)
 opt=(gdiis,calcfc,maxcycle=150,ts,noeigentest) freq=noraman
 #N Geom=AllCheck Guess=Read SCRF=Check GenChk RHF/6-31G(d) Freq
 ---------------------------------------------------------------------------
 Pointgroup= C1   Stoichiometry= C18H24N2O5   C1[X(C18H24N2O5)]  #Atoms= 49
 Charge = 0         Multiplicity = 1
 ---------------------------------------------------------------------------
 SCF Energy= -1178.73199827   Predicted Change= -2.461299D-09
 ===========================================================================
 Optimization completed.            {Found        1        times}
 Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force      0.00000 ||  0.00045   [ YES ]      0.00000 ||  0.00030   [ YES ]
 Displ      0.00336 ||  0.00180   [ NO ]       0.00336 ||  0.00180   [ YES ]
 ---------------------------------------------------------------------------
      Atomic             Coordinates (Angstroms)
       Type           X             Y         Z
 ---------------------------------------------------------------------------
       N        -0.873577       1.418583       1.197189
       C         0.228745       2.382598       1.292159
       C        -0.274398       3.609730       0.524854
       C        -1.797973       3.462553       0.567976
       C        -1.999304       1.949430       0.415339
       C        -0.864575       0.295764       1.884598
       C        -1.776216      -0.737377       1.869110
       C        -0.790109      -1.883133       0.059164
       C        -1.768603      -1.784405       2.961360
       N         0.002817      -1.145974      -0.653687
       C         4.134854      -0.562468      -0.156706
       C         3.385408       0.265385      -0.978288
       C         2.020694       0.058550      -1.116785
       C         1.391947      -0.974328      -0.441337
       C         2.147806      -1.809943       0.377782
       C         3.501118      -1.601294       0.520653
       O         5.459089      -0.447803       0.049047
       C         6.184178       0.547840      -0.619145
       C        -1.994259       1.566169      -1.092289
       O        -3.071942       1.708568      -1.639724
       O        -0.898664       1.211166      -1.575024
       C        -2.174966      -2.203976      -0.433557
       O        -2.595313      -1.325687      -1.289189
       O        -2.745594      -3.176238      -0.057644
       C        -3.907996      -1.437733      -1.838434
       H         1.133299       1.969535       0.866035
       H         0.415768       2.614277       2.336595
       H         0.077894       4.533184       0.969204
       H         0.069191       3.568420      -0.499794
       H        -2.183887       3.793860       1.528225
       H        -2.307638       4.010667      -0.211999
       H        -2.931965       1.622407       0.851420
       H         0.019942       0.165400       2.488709
       H        -2.121740      -2.741145       2.590551
       H        -0.769428      -1.929536       3.365046
       H        -2.415515      -1.509486       3.791201
       H        -0.432294      -0.417680      -1.237481
       H         3.839503       1.073551      -1.517167
       H         1.435399       0.709770      -1.738099
       H         1.702231      -2.636436       0.899072
       H         4.091648      -2.242473       1.147535
       H         6.119911       0.427968      -1.695081
       H         5.839421       1.539057      -0.345006
       H         7.211090       0.430702      -0.308666
       H        -0.390000      -2.604269       0.738361
       H        -2.728218      -0.548216       1.403904
       H        -4.058770      -0.513751      -2.366628
       H        -3.951072      -2.293144      -2.496767
       H        -4.628167      -1.551136      -1.042131
 ---------------------------------------------------------------------------
 Statistical Thermodynamic Analysis
 Temperature= 298.150 Kelvin       Pressure= 1.00000 Atm
 ===========================================================================
 SCF Energy=     -1178.73199827         Predicted Change= -2.461299D-09
 Zero-point correction (ZPE)=      -1178.2944      0.43753
```

```
 Internal Energy (U)=                        -1178.2709      0.46107
 Enthalpy (H)=                               -1178.2699      0.46201
 Gibbs Free Energy (G)=                      -1178.3492      0.38279
---------------------------------------------------------------------------
 Frequencies --  -327.8982               15.3882               31.0796

 Supporting Information: s-Cis-Si-3D-(Methyl-Syn)-(Esther-Syn)2.output
---------------------------------------------------------------------------
 Using  Gaussian 03:  IA32L-G03RevC.02 12-Jun-2004
===========================================================================
 # hf/6-31g(d) scf=(direct,maxcycle=300,tight)
 opt=(gdiis,maxcycle=250,calcfc,ts,noeigentest) freq=noraman
 geom=connectivity
 #N Geom=AllCheck Guess=Read SCRF=Check GenChk RHF/6-31G(d) Freq
---------------------------------------------------------------------------
 Pointgroup= C1   Stoichiometry= C18H24N2O5   C1[X(C18H24N2O5)]  #Atoms= 49
 Charge = 0         Multiplicity = 1
---------------------------------------------------------------------------
 SCF Energy= -1178.72425683   Predicted Change= -7.558432D-09
===========================================================================
 Optimization completed.            {Found        1        times}
 Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force      0.00000 ||  0.00045   [ YES ]      0.00000 ||  0.00030   [ YES ]
 Displ      0.00182 ||  0.00180   [ NO ]       0.00182 ||  0.00180   [ YES ]
---------------------------------------------------------------------------
      Atomic             Coordinates (Angstroms)
       Type           X             Y         Z
---------------------------------------------------------------------------
       N        -0.600339       1.741333       0.940976
       C         0.646564       2.438473       1.272898
       C         0.458802       3.869713       0.729934
       C        -0.921399       3.866832       0.046413
       C        -1.226078       2.393611      -0.224349
       C        -1.124759       0.826682       1.732786
       C        -2.272841       0.079004       1.589078
       C        -1.337815      -1.693108       0.302900
       C        -2.866052      -0.599644       2.807081
       N        -0.413965      -1.283613      -0.504055
       C         3.740404      -1.271731       0.136353
       C         3.169587      -0.512996      -0.873201
       C         1.795740      -0.525134      -1.064882
       C         0.981765      -1.290538      -0.246631
       C         1.556946      -2.064214       0.759032
       C         2.919710      -2.049178       0.950558
       O         5.057209      -1.327497       0.405124
       C         5.957603      -0.590926      -0.376787
       C        -0.550420       1.839284      -1.510278
       O         0.479704       2.393241      -1.861833
       O        -1.093833       0.831317      -2.000529
       C        -2.719288      -1.995324      -0.205869
       O        -2.990150      -1.397471      -1.328703
       O        -3.426834      -2.752352       0.376555
       C        -4.258740      -1.631232      -1.925685
       H         1.480498       1.944618       0.792974
       H         0.798670       2.409529       2.344955
       H         0.504996       4.599483       1.530435
       H         1.232768       4.096004       0.013904
       H        -1.675826       4.271199       0.715292
       H        -0.924832       4.447431      -0.865082
       H        -2.281965       2.170561      -0.239204
       H        -0.523605       0.629043       2.606119
       H        -3.394524      -1.508671       2.545647
       H        -2.093351      -0.861299       3.525908
       H        -3.576264       0.045160       3.320487
       H        -0.716922      -0.683912      -1.285285
       H         3.767075       0.099408      -1.518922
       H         1.366447       0.085025      -1.837192
       H         0.960467      -2.697949       1.388689
       H         3.372671      -2.644348       1.720930
       H         5.919586      -0.897327      -1.416334
       H         5.762070       0.473474      -0.307298
       H         6.939427      -0.799216       0.020159
       H        -1.081907      -2.233653       1.188209
       H        -2.960086       0.371656       0.813805
       H        -4.266287      -1.029910      -2.818711
       H        -4.368957      -2.678383      -2.165866
       H        -5.047171      -1.327313      -1.253086
---------------------------------------------------------------------------
 Statistical Thermodynamic Analysis
 Temperature= 298.150 Kelvin       Pressure= 1.00000 Atm
===========================================================================
 SCF Energy=     -1178.72425683         Predicted Change= -7.558432D-09
 Zero-point correction (ZPE)=      -1178.2868      0.43744
 Internal Energy (U)=                        -1178.2630      0.46118
 Enthalpy (H)=                               -1178.2621      0.46213
 Gibbs Free Energy (G)=                      -1178.3423      0.38188
---------------------------------------------------------------------------
 Frequencies --  -318.9165               19.6659               24.3034

 Supporting Information: s-Cis-Si-3U-(Methyl-Anti)-(Esther-Anti).output
---------------------------------------------------------------------------
 Using  Gaussian 03:  IA32L-G03RevC.02 12-Jun-2004
===========================================================================
 # opt=(calcfc,ts,maxcycle=150,noeigentest) freq=noraman hf/6-31g(d)
 geom=connectivity scf=(direct,tight,maxcycle=300)
 #N Geom=AllCheck Guess=Read SCRF=Check GenChk RHF/6-31G(d) Freq
---------------------------------------------------------------------------
 Pointgroup= C1   Stoichiometry= C18H24N2O5   C1[X(C18H24N2O5)]  #Atoms= 49
 Charge = 0         Multiplicity = 1
---------------------------------------------------------------------------
 SCF Energy= -1178.72375123   Predicted Change= -4.159150D-08
===========================================================================
 Optimization completed.            {Found        1        times}
 Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force      0.00001 ||  0.00045   [ YES ]      0.00000 ||  0.00030   [ YES ]
 Displ      0.00334 ||  0.00180   [ NO ]       0.00334 ||  0.00180   [ YES ]
```

Atomic Type	Coordinates (Angstroms) X	Y	Z
N	-0.563982	1.815911	0.874958
C	0.562483	2.737417	0.770694
C	-0.117457	4.069163	0.476614
C	-1.281731	3.653310	-0.427854
C	-1.735366	2.287104	0.109161
C	-0.552713	0.749973	1.656782
C	-1.527091	-0.211548	1.797449
C	-0.928231	-1.653041	0.038021
C	-1.480975	-1.143516	2.989315
N	-0.088610	-1.120728	-0.797097
C	4.042925	-0.531241	-0.372893
C	3.301950	0.160387	-1.331793
C	1.947835	-0.038529	-1.446782
C	1.295883	-0.943445	-0.606054
C	2.028233	-1.630322	0.341897
C	3.398476	-1.424918	0.464532
O	5.360883	-0.261267	-0.340791
C	6.188576	-0.936086	0.564553
C	-2.095107	1.270960	-1.004790
O	-3.169148	0.696327	-0.879213
O	-1.212903	1.100616	-1.865318
C	-2.293672	-2.000113	-0.537761
O	-3.224175	-2.129839	0.369383
O	-2.400050	-2.243592	-1.688776
C	-4.553706	-2.294512	-0.121794
H	1.212395	2.442665	-0.046285
H	1.140281	2.735648	1.687156
H	-0.483091	4.507213	1.400588
H	0.551864	4.780680	0.007308
H	-2.093916	4.369859	-0.426141
H	-0.936144	3.530579	-1.445539
H	-2.572749	2.375543	0.790390
H	0.363665	0.629485	2.212025
H	-1.908832	-2.113358	2.755346
H	-0.461607	-1.302936	3.335083
H	-2.047527	-0.751783	3.830967
H	-0.506874	-0.544293	-1.527809
H	3.812655	0.851472	-1.975612
H	1.373794	0.509319	-2.171082
H	1.564005	-2.348693	0.991731
H	3.936969	-1.978018	1.208738
H	5.905386	-0.727471	1.590975
H	6.168525	-2.007409	0.395424
H	7.187986	-0.567678	0.390921
H	-0.569455	-2.276527	0.828902
H	-2.491581	-0.011415	1.373247
H	-5.181998	-2.315467	0.753984
H	-4.798637	-1.456345	-0.753967
H	-4.635692	-3.221582	-0.669433

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

SCF Energy= -1178.72375123 Predicted Change= -4.159150D-08
Zero-point correction (ZPE)= -1178.2861 0.43764
Internal Energy (U)= -1178.2626 0.46112
Enthalpy (H)= -1178.2616 0.46206
Gibbs Free Energy (G)= -1178.3403 0.38340

Frequencies -- -383.9040 22.1556 39.3927

Supporting Information: s-Cis-Si-3U-(Methyl-Anti)-(Esther-Syn).output

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

# opt=(calcfc,ts,maxcycle=150,noeigentest) freq=noraman hf/6-31g(d)
geom=check guess=read scf=(direct,tight,maxcycle=300)
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RHF/6-31G(d) Freq

Pointgroup= C1 Stoichiometry= C18H24N2O5 C1[X(C18H24N2O5)] #Atoms= 49
Charge = 0 Multiplicity = 1

SCF Energy= -1178.72974093 Predicted Change= -8.129503D-10

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00062	0.00180	[YES]	0.00062	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
N	-0.765186	1.676164	0.950532
C	0.327781	2.644136	0.946109
C	-0.392696	3.965609	0.708298
C	-1.495002	3.564823	-0.275656
C	-1.911414	2.141214	0.145721
C	-0.790413	0.638361	1.763068
C	-1.738800	-0.356546	1.854297
C	-0.722568	-1.813612	0.293745
C	-1.805071	-1.216131	3.099246
N	-0.009536	-1.197124	-0.597906
C	4.088700	-0.288669	-0.451904
C	3.217355	0.413099	-1.284847
C	1.876569	0.112885	-1.310610
C	1.371725	-0.906377	-0.500634
C	2.235423	-1.612906	0.313185
C	3.590238	-1.302794	0.347919
O	5.379457	0.088010	-0.498824
C	6.330776	-0.584172	0.278136
C	-2.214863	1.268966	-1.099639
O	-3.395994	1.059827	-1.310197

```
      O        -1.213900       0.912845      -1.756289
      C        -2.088844      -2.337909      -0.068787
      O        -2.532730      -1.794150      -1.155181
      O        -2.616580      -3.176317       0.588484
      C        -3.874642      -2.036542      -1.573707
      H         1.014504       2.423546       0.136915
      H         0.874282       2.604293       1.880372
      H        -0.818602       4.325588       1.640096
      H         0.266206       4.732796       0.318720
      H        -2.339837       4.241106      -0.268726
      H        -1.095328       3.534898      -1.281865
      H        -2.786650       2.157607       0.782492
      H         0.076690       0.558751       2.399277
      H        -2.183172      -2.206965       2.878203
      H        -0.824392      -1.324069       3.557517
      H        -2.463852      -0.783403       3.848611
      H        -0.527957      -0.634124      -1.283254
      H         3.616897       1.193574      -1.904775
      H         1.199715       0.664057      -1.936213
      H         1.887978      -2.429717       0.918416
      H         4.232464      -1.872826       0.989999
      H         6.116637      -0.487156       1.337330
      H         6.384083      -1.635325       0.015592
      H         7.279289      -0.116064       0.063968
      H        -0.247150      -2.333684       1.097261
      H        -2.662783      -0.206152       1.320633
      H        -4.079586      -1.266196      -2.293601
      H        -3.942703      -3.026061      -2.002576
      H        -4.541230      -1.950080      -0.730346
 ---------------------------------------------------------------------------
 Statistical Thermodynamic Analysis
 Temperature= 298.150 Kelvin       Pressure= 1.00000 Atm
 ===========================================================================
 SCF Energy=     -1178.72974093         Predicted Change= -8.129503D-10
 Zero-point correction (ZPE)=      -1178.2922      0.43753
 Internal Energy (U)=                      -1178.2686      0.46113
 Enthalpy (H)=                             -1178.2676      0.46207
 Gibbs Free Energy (G)=                    -1178.3471      0.38262
 ---------------------------------------------------------------------------
 Frequencies --  -331.5534                20.1899                30.4895

 Supporting Information: s-Cis-Si-3U-(Methyl-Syn)-(Esther-Anti).output
 ---------------------------------------------------------------------------
 Using  Gaussian 03:  Al64T-G03RevC.01  3-Apr-2004
 ===========================================================================
 # hf/6-31g(d) geom=connectivity scf=(direct,maxcycle=300,tight)
 opt=(maxcycle=250,ts,calcfc,noeigentest) freq=noraman
 #N Geom=AllCheck Guess=Read SCRF=Check GenChk RHF/6-31G(d) Freq
 ---------------------------------------------------------------------------
 Pointgroup= C1   Stoichiometry= C18H24N2O5   C1[X(C18H24N2O5)]  #Atoms= 49
 Charge = 0         Multiplicity = 1
 ---------------------------------------------------------------------------
 SCF Energy= -1178.72410708   Predicted Change= -1.670266D-08
```

```
 ===========================================================================
 Optimization completed.            {Found       1       times}
 Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force      0.00001 ||  0.00045   [ YES ]      0.00000 ||  0.00030   [ YES ]
 Displ      0.00316 ||  0.00180   [ NO ]       0.00316 ||  0.00180   [ YES ]
 ---------------------------------------------------------------------------
      Atomic             Coordinates (Angstroms)
       Type          X             Y         Z
 ---------------------------------------------------------------------------
       N        -0.477105       1.820875       0.875739
       C         0.733591       2.632570       0.830975
       C         0.199946       4.012793       0.467040
       C        -0.934000       3.682423      -0.508774
       C        -1.542184       2.371397       0.014006
       C        -0.615380       0.775537       1.672503
       C        -1.678471      -0.094926       1.755937
       C        -1.078747      -1.625300       0.081929
       C        -1.802884      -0.995997       2.966014
       N        -0.136666      -1.193018      -0.700854
       C         3.990653      -0.961424       0.015476
       C         3.396266      -0.232599      -1.003658
       C         2.027729      -0.317533      -1.210428
       C         1.241018      -1.131602      -0.412876
       C         1.840208      -1.865301       0.607698
       C         3.198128      -1.775802       0.819957
       O         5.305172      -0.949258       0.303963
       C         6.182982      -0.190016      -0.480570
       C        -1.899958       1.363380      -1.108117
       O        -3.026137       0.885258      -1.059563
       O        -0.970541       1.098978      -1.891829
       C        -2.423160      -1.869305      -0.588873
       O        -3.426589      -1.894308       0.246686
       O        -2.465160      -2.132753      -1.739703
       C        -4.724914      -1.959893      -0.341347
       H         1.404766       2.259324       0.064539
       H         1.247885       2.600356       1.783950
       H        -0.185296       4.503656       1.355769
       H         0.961487       4.650130       0.032853
       H        -1.677584       4.467400      -0.571672
       H        -0.533696       3.510611      -1.498902
       H        -2.418451       2.544812       0.626345
       H         0.244612       0.588282       2.295400
       H        -2.299429      -1.929295       2.719819
       H        -0.829729      -1.236844       3.388997
       H        -2.390153      -0.533232       3.755770
       H        -0.447642      -0.603178      -1.472460
       H         3.975079       0.404689      -1.642881
       H         1.562557       0.262952      -1.985646
       H         1.264969      -2.522370       1.233104
       H         3.669700      -2.341379       1.601408
       H         6.165972      -0.511819      -1.516157
       H         5.947169       0.867493      -0.427370
       H         7.168725      -0.354395      -0.073090
```

```
      H        -0.834645      -2.257695       0.908676
      H        -2.587947       0.178871       1.257802
      H        -5.416270      -1.903606       0.483902
      H        -4.849151      -1.121984      -1.008198
      H        -4.845412      -2.891518      -0.873922
--------------------------------------------------------------------------------
 Statistical Thermodynamic Analysis
 Temperature= 298.150 Kelvin       Pressure= 1.00000 Atm
================================================================================
 SCF Energy=     -1178.72410708         Predicted Change= -1.670266D-08
 Zero-point correction (ZPE)=      -1178.2864      0.43768
 Internal Energy (U)=                      -1178.2629      0.46116
 Enthalpy (H)=                             -1178.2619       0.46210
 Gibbs Free Energy (G)=                    -1178.3406       0.38345
--------------------------------------------------------------------------------
 Frequencies --  -388.5692               25.0763               34.1499

 Supporting Information: s-Cis-Si-3U-(Methyl-Syn)-(Esther-Syn).output
--------------------------------------------------------------------------------
 Using  Gaussian 03:  Al64T-G03RevC.01  3-Apr-2004
================================================================================
 #hf/6-31G* scf=(direct,tight,maxcycle=300)
 opt=(gdiis,calcfc,maxcycle=150,ts,noeigentest) freq=noraman
 #N Geom=AllCheck Guess=Read SCRF=Check GenChk RHF/6-31G(d) Freq
--------------------------------------------------------------------------------
 Pointgroup= C1   Stoichiometry= C18H24N2O5   C1[X(C18H24N2O5)]  #Atoms= 49
 Charge = 0         Multiplicity = 1
--------------------------------------------------------------------------------
 SCF Energy= -1178.73011743   Predicted Change= -6.412429D-09
================================================================================
 Optimization completed.             {Found        2        times}
 Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force      0.00001 ||  0.00045   [ YES ]      0.00000 ||  0.00030   [ YES ]
 Displ      0.00149 ||  0.00180   [ YES ]      0.00149 ||  0.00180   [ YES ]
--------------------------------------------------------------------------------
      Atomic             Coordinates (Angstroms)
       Type           X             Y         Z
--------------------------------------------------------------------------------
      N        -0.657293       1.668072       0.979086
      C         0.530103       2.513319       1.046117
      C        -0.033086       3.905240       0.786970
      C        -1.112224       3.631565      -0.264367
      C        -1.691471       2.249077       0.101635
      C        -0.840858       0.636515       1.778262
      C        -1.888746      -0.258164       1.797020
      C        -0.922070      -1.802918       0.301168
      C        -2.126282      -1.107827       3.027862
      N        -0.087620      -1.262293      -0.533212
      C         4.062539      -0.780027      -0.097729
      C         3.341873      -0.010700      -0.998199
      C         1.969384      -0.176965      -1.113524
      C         1.305494      -1.112488      -0.338166
      C         2.032863      -1.894502       0.555802
      C         3.393342      -1.722657       0.678907
      O         5.391493      -0.695763       0.095145
      C         6.151775       0.194226      -0.674688
      C        -1.980615       1.425818      -1.180087
      O        -3.155193       1.350526      -1.492382
      O        -0.971642       0.969708      -1.757802
      C        -2.305692      -2.180859      -0.162673
      O        -2.615485      -1.583021      -1.267445
      O        -2.961384      -2.966227       0.442768
      C        -3.941048      -1.687017      -1.783779
      H         1.231476       2.225656       0.270986
      H         1.017944       2.408365       2.007347
      H        -0.472161       4.299583       1.698469
      H         0.723525       4.602755       0.446862
      H        -1.884820       4.388886      -0.289144
      H        -0.660879       3.579048      -1.247518
      H        -2.606210       2.341936       0.672630
      H        -0.030106       0.467251       2.468887
      H        -2.588745      -2.053947       2.773621
      H        -1.194827      -1.317336       3.549157
      H        -2.785617      -0.610533       3.735469
      H        -0.495076      -0.648267      -1.248148
      H         3.824654       0.721004      -1.615796
      H         1.404146       0.431369      -1.794516
      H         1.556987      -2.655157       1.146518
      H         3.962715      -2.323313       1.362928
      H         6.076003      -0.034249      -1.732176
      H         5.849207       1.222010      -0.504965
      H         7.175143       0.068519      -0.355872
      H        -0.561116      -2.375439       1.128221
      H        -2.755089      -0.012764       1.205034
      H        -4.016588      -0.893253      -2.503518
      H        -4.075143      -2.660712      -2.232811
      H        -4.655036      -1.543470      -0.988246
--------------------------------------------------------------------------------
 Statistical Thermodynamic Analysis
 Temperature= 298.150 Kelvin       Pressure= 1.00000 Atm
================================================================================
 SCF Energy=     -1178.73011743         Predicted Change= -6.412429D-09
 Zero-point correction (ZPE)=      -1178.2925      0.43757
 Internal Energy (U)=                      -1178.2689      0.46117
 Enthalpy (H)=                             -1178.2679       0.46211
 Gibbs Free Energy (G)=                    -1178.3474       0.38266
--------------------------------------------------------------------------------
 Frequencies --  -336.4616               22.4299               29.0862
```

ii. Pipecolinic Acid Transition Structures.

```
 Supporting Information: Pipecolinic-Acid-TS-s-Trans-Re.output
--------------------------------------------------------------------------------
 Using  Gaussian 03:  Al64T-G03RevC.01  3-Apr-2004
```

```
 ============================================================================
 # opt=(calcfc,gdiis,ts,noeigentest,maxcycle=250) hf/6-31G* freq=noraman
 #N Geom=AllCheck Guess=Read SCRF=Check GenChk RHF/6-31G(d) Freq
 ----------------------------------------------------------------------------
 Pointgroup= C1   Stoichiometry= C19H26N2O5   C1[X(C19H26N2O5)]  #Atoms= 52
 Charge = 0         Multiplicity = 1
 ----------------------------------------------------------------------------
 SCF Energy= -1217.76421776   Predicted Change= -5.366109D-09
 ============================================================================
 Optimization completed.            {Found        1        times}
 Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force      0.00001 ||  0.00045   [ YES ]      0.00000 ||  0.00030   [ YES ]
 Displ      0.00228 ||  0.00180   [ NO ]       0.00228 ||  0.00180   [ YES ]
 ----------------------------------------------------------------------------
       Atomic             Coordinates (Angstroms)
        Type           X             Y         Z
 ----------------------------------------------------------------------------
       C         3.290076       3.253638       0.125697
       C         1.908400       3.395331       0.761495
       C         1.058345       2.142795       0.540460
       C         3.127047       0.754525       0.444911
       C         3.980912       2.002099       0.663841
       H         0.170076       2.222538       1.155163
       H         2.021592       3.567182       1.830126
       H         1.368845       4.233194       0.343104
       H         3.191514       3.186052      -0.954599
       H         3.891518       4.133187       0.334862
       H         3.587720      -0.088086       0.938738
       H         3.035644       0.534709      -0.609531
       H         4.175251       2.120774       1.727305
       H         4.940738       1.848573       0.178313
       N         1.780467       0.937469       0.986092
       C         0.540311       2.036420      -0.928239
       O        -0.113260       2.996087      -1.292482
       O         0.802043       0.986690      -1.548831
       C         1.130006      -0.017489       1.618269
       C         1.460731      -1.344573       1.826875
       H         2.457907      -1.671036       1.592851
       C         0.780930      -2.128060       2.930166
       H         0.758849      -3.189913       2.700143
       H         1.299341      -2.027933       3.881069
       H        -0.243223      -1.798333       3.084073
       H         0.157801       0.289626       1.967102
       C         0.294692      -2.154085      -0.067351
       H        -0.184376      -2.833115       0.602495
       C         1.572439      -2.689682      -0.646258
       N        -0.411601      -1.281513      -0.716571
       H         0.097508      -0.599861      -1.289419
       C        -1.746614      -0.902683      -0.411500
       C        -2.567218      -1.640865       0.439994
       C        -2.248514       0.237864      -1.015040
       C        -3.855099      -1.227648       0.690085
       H        -2.223573      -2.544222       0.908131
       C        -3.547425       0.654419      -0.762183
       H        -1.628657       0.818493      -1.671077
       C        -4.358193      -0.072519       0.093525
       H        -4.494538      -1.789998       1.344089
       H        -3.894631       1.549960      -1.237757
       O        -5.626111       0.245613       0.407616
       C        -6.210408       1.394789      -0.143625
       H        -6.256417       1.333404      -1.225316
       H        -7.212985       1.440908       0.253325
       H        -5.669352       2.289207       0.144382
       O         2.008243      -3.737445      -0.296449
       O         2.076508      -1.915344      -1.566201
       C         3.263563      -2.345540      -2.220566
       H         3.490889      -1.573338      -2.935838
       H         4.064748      -2.451853      -1.504126
       H         3.092478      -3.289038      -2.716810
 ----------------------------------------------------------------------------
 Statistical Thermodynamic Analysis
 Temperature= 298.150 Kelvin       Pressure= 1.00000 Atm
 ============================================================================
 SCF Energy=     -1217.76421776         Predicted Change= -5.366109D-09
 Zero-point correction (ZPE)=      -1217.2950      0.46913
 Internal Energy (U)=                      -1217.2706      0.49360
 Enthalpy (H)=                             -1217.2696       0.49454
 Gibbs Free Energy (G)=                    -1217.3512       0.41295
 ----------------------------------------------------------------------------
 Frequencies --  -330.0387               16.0619               32.0403

 Supporting Information: Pipecolinic-Acid-TS-s-Trans-Re2.output
 ----------------------------------------------------------------------------
 Using  Gaussian 03:  Al64T-G03RevC.01  3-Apr-2004
 ============================================================================
 # opt=(calcfc,ts,maxcycle=150,noeigentest) freq=noraman hf/6-31g(d)
 geom=connectivity scf=(direct,tight,maxcycle=300)
 #N Geom=AllCheck Guess=Read SCRF=Check GenChk RHF/6-31G(d) Freq
 ----------------------------------------------------------------------------
 Pointgroup= C1   Stoichiometry= C19H26N2O5   C1[X(C19H26N2O5)]  #Atoms= 52
 Charge = 0         Multiplicity = 1
 ----------------------------------------------------------------------------
 SCF Energy= -1217.76278775   Predicted Change= -9.060687D-09
 ============================================================================
 Optimization completed.            {Found        2        times}
 Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force      0.00004 ||  0.00045   [ YES ]      0.00000 ||  0.00030   [ YES ]
 Displ      0.00179 ||  0.00180   [ YES ]      0.00179 ||  0.00180   [ YES ]
 ----------------------------------------------------------------------------
       Atomic             Coordinates (Angstroms)
        Type           X             Y         Z
 ----------------------------------------------------------------------------
       C         2.876590       3.665036       0.044365
       C         1.542891       3.615919       0.787931
       C         0.807927       2.297852       0.534357
       C         2.989663       1.147100       0.178232
```

C	3.730906	2.458646	0.430023
H	-0.035167	2.242116	1.211958
H	1.723128	3.725120	1.855819
H	0.890343	4.418556	0.474751
H	2.698559	3.662963	-1.027656
H	3.401741	4.586647	0.277123
H	3.571431	0.322256	0.560155
H	2.826475	0.992919	-0.878154
H	4.001065	2.523270	1.481892
H	4.656511	2.441363	-0.138494
N	1.682352	1.151102	0.841202
C	0.194001	2.238209	-0.900401
O	-0.574940	3.148880	-1.143884
O	0.511394	1.268970	-1.617991
C	1.208738	0.121533	1.508673
C	1.704266	-1.162322	1.656269
H	2.717607	-1.359434	1.355252
C	1.185527	-2.048654	2.768371
H	1.235354	-3.099243	2.492390
H	1.763813	-1.941448	3.683685
H	0.151455	-1.820275	3.012364
H	0.241144	0.307157	1.945168
C	0.523907	-2.004492	-0.248400
H	0.142846	-2.768002	0.393159
C	1.840177	-2.290995	-0.908479
N	-0.284139	-1.167008	-0.809395
H	0.128142	-0.407737	-1.368351
C	-1.639568	-0.947751	-0.442798
C	-2.313428	-1.741378	0.484217
C	-2.312384	0.094815	-1.057860
C	-3.630486	-1.484945	0.787323
H	-1.831259	-2.564236	0.977706
C	-3.639255	0.354671	-0.749869
H	-1.798779	0.723551	-1.759345
C	-4.307218	-0.431829	0.174196
H	-4.157526	-2.090368	1.500445
H	-4.120600	1.180032	-1.235269
O	-5.588342	-0.263080	0.544355
C	-6.337846	0.786148	-0.006934
H	-6.432107	0.680544	-1.082048
H	-7.316480	0.724087	0.443955
H	-5.896808	1.749275	0.223988
O	2.333321	-1.609939	-1.739429
O	2.327252	-3.431337	-0.464567
C	3.570080	-3.854485	-1.012314
H	3.792071	-4.795654	-0.536636
H	3.483174	-3.979585	-2.081060
H	4.339966	-3.128953	-0.794732

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

SCF Energy= -1217.76278775 Predicted Change= -9.060687D-09

Zero-point correction (ZPE)= -1217.2938 0.46893
Internal Energy (U)= -1217.2694 0.49337
Enthalpy (H)= -1217.2684 0.49431
Gibbs Free Energy (G)= -1217.3498 0.41290

Frequencies -- -306.4482 16.8712 31.1788

Supporting Information: Pipecolinic-Acid-TS-s-Trans-Si.output

---

Using Gaussian 03: Al64T-G03RevC.01 3-Apr-2004

---

opt=(gdiis,maxcycle=300,ts,calcfc,noeigentest) hf/6-31G* freq=noraman
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RHF/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C19H26N2O5 C1[X(C19H26N2O5)] #Atoms= 52
Charge = 0 Multiplicity = 1

SCF Energy= -1217.76570246 Predicted Change= -5.088931D-08

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00001	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00571	0.00180	[NO]	0.00571	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.923314	4.061285	0.873216
C	-2.207963	3.497875	0.263936
C	-1.978660	2.108946	-0.335473
C	-0.131343	1.696027	1.250200
C	-0.323516	3.076616	1.879352
H	-2.930748	1.678285	-0.621470
H	-2.974581	3.426974	1.034731
H	-2.573362	4.147505	-0.517236
H	-0.211607	4.254428	0.076490
H	-1.123728	5.012295	1.357892
H	0.226856	0.990675	1.983154
H	0.596494	1.745610	0.452418
H	-0.977427	2.984216	2.743957
H	0.638099	3.431172	2.240743
N	-1.394700	1.220652	0.686282
C	-1.132832	2.143372	-1.654192
O	-1.285435	3.135259	-2.333480
O	-0.420677	1.142604	-1.887829
C	-2.057090	0.170349	1.128512
C	-1.607590	-0.916344	1.852156
H	-0.630627	-0.872188	2.301135
C	-2.589529	-1.850756	2.523468
H	-2.235307	-2.877598	2.519918
H	-2.758951	-1.576844	3.562373
H	-3.554961	-1.840000	2.026498
H	-3.069164	0.119378	0.767265

C	-0.743390	-1.926404	-0.087822
H	-0.385301	-2.730669	0.519009
C	-2.080364	-2.148187	-0.732363
N	0.090539	-1.107448	-0.636465
H	-0.272467	-0.322079	-1.224454
C	1.472679	-1.017244	-0.329134
C	2.072670	-1.717200	0.714867
C	2.250419	-0.194230	-1.127064
C	3.425961	-1.600366	0.940843
H	1.501178	-2.351843	1.366184
C	3.612793	-0.074644	-0.898390
H	1.782076	0.367888	-1.912626
C	4.210704	-0.779830	0.134734
H	3.896798	-2.135925	1.743586
H	4.183938	0.572204	-1.534648
O	5.520212	-0.735403	0.439221
C	6.383967	0.066264	-0.319294
H	6.104442	1.112526	-0.261520
H	7.366455	-0.063497	0.108167
H	6.401988	-0.245685	-1.357805
O	-2.621645	-1.378167	-1.449505
O	-2.538669	-3.338274	-0.406820
C	-3.790551	-3.720840	-0.965879
H	-3.983156	-4.713855	-0.594367
H	-4.565368	-3.039637	-0.647200
H	-3.731021	-3.722047	-2.043653

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1217.76570246 Predicted Change= -5.088931D-08
Zero-point correction (ZPE)= -1217.2969 0.46872
Internal Energy (U)= -1217.2727 0.49294
Enthalpy (H)= -1217.2718 0.49388
Gibbs Free Energy (G)= -1217.3519 0.41374

Frequencies -- -317.0773 28.8534 32.5125

Supporting Information: Pipecolinic-Acid-TS-s-Trans-Si2.output

---

Using Gaussian 03: Al64T-G03RevC.01 3-Apr-2004

==========

# opt=(calcfc,ts,maxcycle=150,noeigentest) freq=noraman hf/6-31g(d)
geom=connectivity scf=(direct,tight,maxcycle=300)
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RHF/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C19H26N2O5 C1[X(C19H26N2O5)] #Atoms= 52
Charge = 0 Multiplicity = 1

SCF Energy= -1217.76997963 Predicted Change= -5.192499D-08

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00003	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00386	0.00180	[NO]	0.00386	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-1.342410	3.802555	0.608515
C	-2.664163	3.081224	0.352181
C	-2.452217	1.597858	0.032187
C	-0.342093	1.629896	1.407058
C	-0.589158	3.100591	1.736509
H	-3.412533	1.102813	0.078860
H	-3.292916	3.167527	1.236232
H	-3.201521	3.522415	-0.477300
H	-0.738388	3.800796	-0.294131
H	-1.527962	4.840203	0.869523
H	0.077924	1.129738	2.267513
H	0.353735	1.552531	0.586468
H	-1.160832	3.174279	2.658955
H	0.372178	3.573755	1.916353
N	-1.591691	0.955827	1.046282
C	-1.942917	1.404263	-1.428865
O	-2.801538	1.579523	-2.273019
O	-0.737893	1.109807	-1.580043
C	-1.910028	-0.250661	1.483743
C	-1.122337	-1.220812	2.067205
H	-0.116672	-0.965663	2.353938
C	-1.749607	-2.374439	2.817202
H	-1.156894	-3.280258	2.726738
H	-1.838990	-2.158732	3.879389
H	-2.740934	-2.604433	2.442822
H	-2.930390	-0.526779	1.276334
C	-0.395572	-2.066837	0.018806
H	0.084970	-2.835825	0.584824
C	-1.743554	-2.464123	-0.516276
N	0.308137	-1.166585	-0.592308
H	-0.190546	-0.443420	-1.135011
C	1.680908	-0.890279	-0.379977
C	2.477445	-1.597960	0.517064
C	2.243631	0.132333	-1.124927
C	3.810501	-1.283778	0.654658
H	2.077376	-2.395182	1.115129
C	3.586694	0.449223	-0.986443
H	1.624953	0.689432	-1.803334
C	4.379759	-0.258224	-0.096633
H	4.433122	-1.823936	1.342664
H	3.989511	1.246967	-1.578724
O	5.689004	-0.033205	0.113643
C	6.346931	0.972857	-0.606532
H	5.919505	1.948561	-0.402455
H	7.373396	0.957827	-0.273569
H	6.314311	0.780267	-1.673321
O	-2.219383	-3.520447	-0.256789

```
      O        -2.256758      -1.545166      -1.282048
      C        -3.497611      -1.793406      -1.945015
      H        -3.712023      -0.879571      -2.470904
      H        -3.384668      -2.625227      -2.624144
      H        -4.263504      -2.018545      -1.217368
---------------------------------------------------------------------------
 Statistical Thermodynamic Analysis
 Temperature= 298.150 Kelvin       Pressure= 1.00000 Atm
===========================================================================
 SCF Energy=     -1217.76997963         Predicted Change= -5.192499D-08
 Zero-point correction (ZPE)=      -1217.3006      0.46928
 Internal Energy (U)=                      -1217.2764      0.49356
 Enthalpy (H)=                             -1217.2754      0.49450
 Gibbs Free Energy (G)=                    -1217.3553      0.41465
---------------------------------------------------------------------------
 Frequencies --  -320.7281               31.3717               32.6586

 Supporting Information: Pipecolinic-Acid-TS-s-Cis-Re.output
---------------------------------------------------------------------------
 Using  Gaussian 03:  Al64T-G03RevC.01  3-Apr-2004
===========================================================================
 # opt=(gdiis,maxcycle=300,ts,calcfc,noeigentest) hf/6-31G* freq=noraman
 #N Geom=AllCheck Guess=Read SCRF=Check GenChk RHF/6-31G(d) Freq
---------------------------------------------------------------------------
 Pointgroup= C1   Stoichiometry= C19H26N2O5   C1[X(C19H26N2O5)]  #Atoms= 52
 Charge = 0         Multiplicity = 1
---------------------------------------------------------------------------
 SCF Energy= -1217.76593061   Predicted Change= -2.071789D-08
===========================================================================
 Optimization completed.           {Found       1       times}
 Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force      0.00004 ||  0.00045   [ YES ]      0.00000 ||  0.00030   [ YES ]
 Displ      0.00267 ||  0.00180   [ NO ]       0.00267 ||  0.00180   [ YES ]
---------------------------------------------------------------------------
      Atomic             Coordinates (Angstroms)
       Type           X             Y         Z
---------------------------------------------------------------------------
      C        -4.077379      -2.674330      -0.553438
      C        -2.716247      -3.018787       0.046028
      C        -1.839777      -1.779771       0.263327
      C        -3.916122      -0.403054       0.495073
      C        -4.778873      -1.648113       0.333957
      H        -1.018468      -2.082111       0.897784
      H        -2.868498      -3.512869       1.003116
      H        -2.164377      -3.697497      -0.590383
      H        -3.951554      -2.269217      -1.554596
      H        -4.681854      -3.571633      -0.647386
      H        -4.367273       0.281984       1.202082
      H        -3.825658       0.107152      -0.455787
      H        -4.978565      -2.083087       1.310606
      H        -5.735058      -1.353851      -0.089796
      N        -2.571728      -0.732038       0.976490
      C        -1.188745      -1.271638      -1.047132
      O        -0.408649      -2.057526      -1.568385
      O        -1.459831      -0.108650      -1.402829
      C        -1.935582       0.157357       1.727581
      C        -0.591427       0.301522       1.993703
      H         0.092658      -0.460505       1.665854
      C        -0.171921       1.076138       3.227332
      H        -0.190039       0.462807       4.125487
      H         0.844248       1.452692       3.137424
      H        -0.824212       1.927921       3.399515
      H        -2.587444       0.887658       2.170426
      C         0.093211       1.775168       0.275777
      H         0.575544       2.248291       1.104464
      C        -1.183275       2.440632      -0.214287
      N         0.806066       1.104867      -0.573213
      H         0.265231       0.684462      -1.322346
      C         2.129582       0.637103      -0.356293
      C         3.091653       1.449089       0.236716
      C         2.464155      -0.637425      -0.772893
      C         4.366897       0.974059       0.435611
      H         2.854904       2.458324       0.522743
      C         3.754631      -1.113391      -0.582541
      H         1.718567      -1.263879      -1.231676
      C         4.708989      -0.314690       0.027485
      H         5.121740       1.588497       0.888792
      H         3.987698      -2.106668      -0.911695
      O         5.981286      -0.682833       0.261378
      C         6.421148      -1.954679      -0.129348
      H         6.336887      -2.089129      -1.202142
      H         7.460355      -2.013351       0.156191
      H         5.866644      -2.737101       0.377081
      O        -2.081042       2.743231       0.498103
      O        -1.076282       2.748348      -1.477865
      C        -2.243072       3.231333      -2.132016
      H        -1.940586       3.435489      -3.145682
      H        -3.003420       2.466209      -2.113171
      H        -2.598769       4.129920      -1.650906
---------------------------------------------------------------------------
 Statistical Thermodynamic Analysis
 Temperature= 298.150 Kelvin       Pressure= 1.00000 Atm
===========================================================================
 SCF Energy=     -1217.76593061         Predicted Change= -2.071789D-08
 Zero-point correction (ZPE)=      -1217.2964      0.46945
 Internal Energy (U)=                      -1217.2721      0.49375
 Enthalpy (H)=                             -1217.2712      0.49470
 Gibbs Free Energy (G)=                    -1217.3521      0.41381
---------------------------------------------------------------------------
 Frequencies --  -345.0952               20.5232               30.2146

 Supporting Information: Pipecolinic-Acid-TS-s-Cis-Re2-R.output
---------------------------------------------------------------------------
 Using  Gaussian 03:  Al64T-G03RevC.01  3-Apr-2004
===========================================================================
 # fopt=(calcfc,ts,maxcycle=150,noeigentest,gdiis) freq=noraman hf/6-31g(d)
```

```
 scf=(direct,tight,maxcycle=300)
 #N Geom=AllCheck Guess=Read SCRF=Check GenChk RHF/6-31G(d) Freq
--------------------------------------------------------------------------------
 Pointgroup= C1   Stoichiometry= C19H26N2O5   C1[X(C19H26N2O5)]  #Atoms= 52
 Charge = 0         Multiplicity = 1
--------------------------------------------------------------------------------
 SCF Energy= -1217.76351487   Predicted Change= -9.678852D-09
================================================================================
 Optimization completed.            {Found        2        times}
 Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force      0.00004 ||  0.00045   [ YES ]      0.00000 ||  0.00030   [ YES ]
 Displ      0.00139 ||  0.00180   [ YES ]      0.00139 ||  0.00180   [ YES ]
--------------------------------------------------------------------------------
      Atomic             Coordinates (Angstroms)
       Type           X             Y         Z
--------------------------------------------------------------------------------
       C        -3.463297      -3.409885      -0.097639
       C        -2.313512      -3.208810       0.887710
       C        -1.542488      -1.911910       0.615527
       C        -3.613867      -0.913541      -0.337895
       C        -4.392048      -2.196630      -0.068250
       H        -0.874384      -1.749062       1.449438
       H        -2.711177      -3.178888       1.900292
       H        -1.605077      -4.022958       0.830820
       H        -3.066668      -3.545586      -1.100441
       H        -4.014619      -4.312191       0.149744
       H        -4.252773      -0.047878      -0.212012
       H        -3.230548      -0.902087      -1.349279
       H        -4.876538      -2.129277       0.903583
       H        -5.176750      -2.289102      -0.813916
       N        -2.471799      -0.776790       0.572622
       C        -0.633556      -2.018246      -0.641288
       O         0.139615      -2.962634      -0.623224
       O        -0.743572      -1.118577      -1.493800
       C        -2.214760       0.390818       1.126637
       C        -1.058794       0.884986       1.706047
       H        -0.222804       0.219279       1.831531
       C        -1.161414       2.003314       2.723476
       H        -1.319607       1.618931       3.728683
       H        -0.254299       2.600657       2.760754
       H        -1.982176       2.676469       2.498618
       H        -3.048967       1.073774       1.086695
       C        -0.036266       1.910035      -0.152849
       H         0.438955       2.537272       0.570446
       C        -1.296283       2.440135      -0.774875
       N         0.668177       1.048607      -0.810182
       H         0.150389       0.382469      -1.394355
       C         2.008017       0.692441      -0.490950
       C         2.909051       1.638881      -0.007745
       C         2.430164      -0.606958      -0.707214
       C         4.200835       1.276046       0.292309
       H         2.617249       2.666716       0.112542
       C         3.736366      -0.970981      -0.409824
       H         1.753392      -1.348700      -1.087999
       C         4.625366      -0.037654       0.097506
       H         4.905239       1.996860       0.662507
       H         4.028742      -1.988594      -0.576723
       O         5.906024      -0.292732       0.419624
       C         6.421820      -1.584322       0.244982
       H         6.384595      -1.886565      -0.795769
       H         7.451207      -1.542009       0.566970
       H         5.886921      -2.308030       0.849890
       O        -1.831345       1.962865      -1.714311
       O        -1.678601       3.540847      -0.157724
       C        -2.831645       4.196030      -0.671100
       H        -2.972610       5.065918      -0.050702
       H        -2.670113       4.484297      -1.698917
       H        -3.691330       3.544935      -0.611400
--------------------------------------------------------------------------------
 Statistical Thermodynamic Analysis
 Temperature= 298.150 Kelvin       Pressure= 1.00000 Atm
================================================================================
 SCF Energy=     -1217.76351487         Predicted Change= -9.678852D-09
 Zero-point correction (ZPE)=      -1217.2946      0.46885
 Internal Energy (U)=                      -1217.2702      0.49326
 Enthalpy (H)=                             -1217.2693      0.49420
 Gibbs Free Energy (G)=                    -1217.3504      0.41306
--------------------------------------------------------------------------------
 Frequencies --  -319.4486               20.5595               31.1478

 Supporting Information: Pipecolinic-Acid-TS-s-Cis-Si.output
--------------------------------------------------------------------------------
 Using  Gaussian 03:  Al64T-G03RevC.01  3-Apr-2004
================================================================================
 # opt=(gdiis,maxcycle=300,ts,calcfc,noeigentest) hf/6-31G* freq=noraman
 #N Geom=AllCheck Guess=Read SCRF=Check GenChk RHF/6-31G(d) Freq
--------------------------------------------------------------------------------
 Pointgroup= C1   Stoichiometry= C19H26N2O5   C1[X(C19H26N2O5)]  #Atoms= 52
 Charge = 0         Multiplicity = 1
--------------------------------------------------------------------------------
 SCF Energy= -1217.76936200   Predicted Change= -8.067874D-09
================================================================================
 Optimization completed.            {Found        2        times}
 Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force      0.00001 ||  0.00045   [ YES ]      0.00000 ||  0.00030   [ YES ]
 Displ      0.00179 ||  0.00180   [ YES ]      0.00179 ||  0.00180   [ YES ]
--------------------------------------------------------------------------------
      Atomic             Coordinates (Angstroms)
       Type           X             Y         Z
--------------------------------------------------------------------------------
       C        -1.793376       3.868424       0.350005
       C        -2.808213       2.732285       0.474883
       C        -2.190003       1.366961       0.142864
       C         0.024240       2.216570       0.870339
       C        -0.566740       3.580636       1.216576
       H        -2.906906       0.608810       0.412837
```

H	-3.191659	2.705568	1.493279
H	-3.644074	2.884230	-0.192915
H	-1.491134	3.974364	-0.688692
H	-2.248972	4.809315	0.643815
H	0.843406	1.969879	1.533494
H	0.398900	2.217748	-0.143358
H	-0.844759	3.598786	2.268336
H	0.197108	4.339833	1.072207
N	-0.987326	1.161142	0.967024
C	-1.958828	1.188479	-1.393850
O	-2.963615	1.361967	-2.057181
O	-0.812897	0.868300	-1.772010
C	-0.817423	0.146538	1.794594
C	-1.558226	-1.005328	1.950601
H	-2.556551	-1.032121	1.553964
C	-1.307458	-1.928036	3.122490
H	-1.947003	-1.694861	3.970779
H	-1.507623	-2.961607	2.854832
H	-0.278193	-1.867006	3.467247
H	0.095334	0.207501	2.363773
C	-0.498355	-2.104471	0.121037
H	-0.030814	-2.780852	0.803557
C	-1.855535	-2.547789	-0.348135
N	0.216859	-1.303680	-0.600473
H	-0.273012	-0.638491	-1.222243
C	1.581268	-0.990884	-0.387812
C	2.344699	-1.540992	0.638802
C	2.171536	-0.095837	-1.264916
C	3.672836	-1.201428	0.772256
H	1.923477	-2.235334	1.341385
C	3.508086	0.246049	-1.131717
H	1.577733	0.345938	-2.042561
C	4.269006	-0.306662	-0.112318
H	4.270032	-1.621994	1.559212
H	3.932438	0.941679	-1.828503
O	5.569563	-0.043025	0.105339
C	6.255696	0.832021	-0.747707
H	5.825489	1.827304	-0.721741
H	7.270046	0.873768	-0.381680
H	6.258726	0.466283	-1.768653
O	-2.325605	-3.572043	0.026356
O	-2.378297	-1.705838	-1.188939
C	-3.659372	-1.977450	-1.757709
H	-3.897676	-1.093836	-2.323036
H	-3.596874	-2.850859	-2.389826
H	-4.380373	-2.145679	-0.971574

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1217.76936200 Predicted Change= -8.067874D-09
Zero-point correction (ZPE)= -1217.3003 0.46904
Internal Energy (U)= -1217.2760 0.49331
Enthalpy (H)= -1217.2750 0.49426
Gibbs Free Energy (G)= -1217.3550 0.41431

Frequencies -- -309.8659 29.9834 33.3325

Supporting Information: Pipecolinic-Acid-TS-s-Cis-Si2.output

Using Gaussian 03: Al64T-G03RevC.01 3-Apr-2004

==========

# opt=(calcfc,ts,maxcycle=150,noeigentest) freq=noraman hf/6-31g(d)
geom=connectivity scf=(direct,tight,maxcycle=300)
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RHF/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C19H26N2O5 C1[X(C19H26N2O5)] #Atoms= 52
Charge = 0 Multiplicity = 1

SCF Energy= -1217.76366569 Predicted Change= -8.569846D-09

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00005	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00139	0.00180	[YES]	0.00139	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-1.568110	4.045689	0.612430
C	-2.602163	2.931572	0.431951
C	-1.960071	1.652616	-0.115874
C	0.185591	2.262310	0.917761
C	-0.386661	3.570351	1.463240
H	-2.692841	0.860180	-0.129213
H	-3.071324	2.706784	1.389113
H	-3.372773	3.245243	-0.256511
H	-1.216592	4.354345	-0.366024
H	-2.030484	4.913176	1.074224
H	0.965843	1.875290	1.560408
H	0.610158	2.407904	-0.066251
H	-0.707240	3.413928	2.491625
H	0.399702	4.320002	1.483528
N	-0.869839	1.254511	0.796305
C	-1.477937	1.797496	-1.602256
O	-2.094731	2.600147	-2.266505
O	-0.532733	1.054863	-1.948984
C	-0.910681	0.237832	1.630679
C	-1.790872	-0.825420	1.689782
H	-2.753778	-0.710777	1.225531
C	-1.745976	-1.778210	2.864470
H	-2.433322	-1.485291	3.655067
H	-2.021283	-2.785614	2.566336
H	-0.752057	-1.825333	3.301731
H	-0.059942	0.191185	2.290285
C	-0.736145	-1.942865	-0.097320

H	-0.371780	-2.693804	0.570364
C	-2.090052	-2.193878	-0.692948
N	0.090221	-1.182045	-0.736610
H	-0.290897	-0.430200	-1.355867
C	1.462199	-1.025616	-0.424535
C	2.082992	-1.657144	0.650151
C	2.213998	-0.202853	-1.249371
C	3.429391	-1.473704	0.881210
H	1.535523	-2.294844	1.318778
C	3.567160	-0.017563	-1.017329
H	1.730643	0.307526	-2.060319
C	4.185702	-0.654739	0.048849
H	3.915555	-1.959066	1.706487
H	4.117064	0.625629	-1.675725
O	5.489924	-0.541913	0.359768
C	6.328699	0.251811	-0.434051
H	6.012549	1.289283	-0.428575
H	7.312942	0.178091	0.002593
H	6.363105	-0.109512	-1.456017
O	-2.587705	-1.523484	-1.530262
O	-2.619029	-3.282075	-0.171483
C	-3.906978	-3.658123	-0.646619
H	-4.160276	-4.560977	-0.115451
H	-4.624448	-2.879171	-0.435308
H	-3.873033	-3.838911	-1.710256

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

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SCF Energy= -1217.76366569 Predicted Change= -8.569846D-09
Zero-point correction (ZPE)= -1217.2951 0.46853
Internal Energy (U)= -1217.2708 0.49277
Enthalpy (H)= -1217.2699 0.49371
Gibbs Free Energy (G)= -1217.3500 0.41362

Frequencies -- -341.0823 30.0428 36.1660