Asymmetric Synthesis of a (2*Z*,7*E*)-Cyclononadiene by an Intramolecular Cycloalkylation and Insight to Its Conformational Properties

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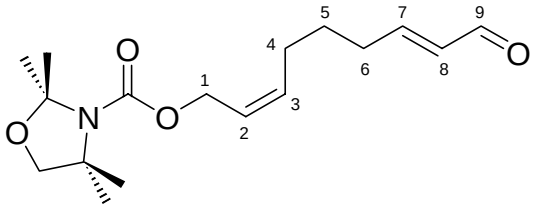
Supporting Information:

1. Detailed reaction procedures and analytical data

(2*Z*,7*E*)-9-Oxo-2,7-nonadienyl 2,2,4,4-tetramethyl-1,3-oxazolidine-3-carboxylate



The allylic alcohol **1** (670 mg, 2.15 mmol, 1.0 equiv.) was introduced at room temperature to a suspension of PCC (557 mg, 2.58 mmol, 1.2 equiv.) in CH_2Cl_2 (15 ml) and stirred for 3 hrs. After filtration over silica gel and evaporation of the solvent in vacuo, the crude product (after measuring a ^1H and a ^{13}C NMR spectra) has been used in the next step without further purifications.

t_R = 19.05 min (HP1; 50°C, 10°C/min, 290°C, 10 min); R_f = 0.35 (ether/pentane = 1:1); colorless liquid.

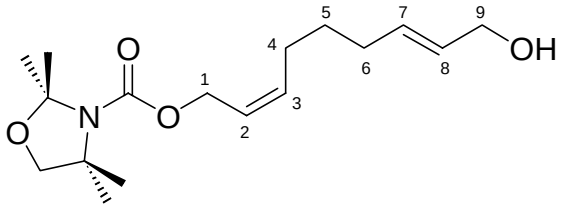
^1H NMR (300 MHz, $CDCl_3$): δ / ppm = 1.33, 1.39 (s, 6 H, CH_3(*Cby*)); 1.49, 1.53 (s, 6 H, CH_3(*Cby*)); 1.59 (quin., 2 H, H-5); 2.13-2.20 (m, 2 H, H-4); 2.32 (dq, 2 H, H-6); 3.69 (s, 2 H, CH_2(*Cby*)); 4.61 (d, 2 H, H-1); 5.56-5.59 (m, 2 H, H-2, H-3); 6.09 (ddt, 1 H, H-8); 6.80 (dt, 1 H, H-7); 9.48 (d, 1 H, H-9).

$^3J_{1,2}$ = 5.4 Hz, $^3J_{4,5}$ = $^3J_{5,6}$ = 10.2 Hz, $^3J_{6,7}$ = 7.4 Hz, $^4J_{6,8}$ = 1.3 Hz, $^3J_{7,8}$ = 15.5 Hz, $^3J_{8,9}$ = 7.8 Hz.

The coupling constant $^3J_{7,8}$ = 15.5 Hz clearly shows the *E* configuration for the 7-8 double bond.

^{13}C NMR (90 MHz, $CDCl_3$): δ / ppm = 24.1, 25.2, 26.4 (CH_3(*Cby*)); 26.9, 27.5 (C-4, C-5); 32.0 (C-6); 59.7, 60.6 (C(*Cby*)); 60.0 (C-1); 76.1, 76.5 (CH_2(*Cby*)); 94.8, 95.8 (C(*Cby*)); 125.1 133.1, 133.2 (C-2, C-3, C-8); 152.4 (C=O(*Cby*)); 157.9 (C-7); 198.8 (C-9).

(2*Z*,7*E*)-9-Hydroxy-2,7-nonadienyl 2,2,4,4-tetramethyl-1,3-oxazolidine-3-carboxylate (2)



The crude product (645 mg, 2.08 mmol, 1.0 equiv.) of the previous step has been dissolved in THF (5 ml) and cooled to –78°C. After injection of DIBAH (2.7 ml, 2.71 mmol, 1.3 equiv., 1 M solution in heptane) within 10 min the reaction mixture was stirred for further 40 min. Then, methanol (2 ml) and water (0.5 ml) were added and the reaction mixture was allowed to warm up to room temperature. After drying ($MgSO_4$), filtration and evaporation of the solvent, the crude product was purified by flash chromatography over silica gel (diethyl ether). The product **2** (620 mg) was obtained in 93% yield (over the last two steps).

t_R = 23.64 min (HP1701; 50°C, 10°C/min, 260°C, 10 min); R_f = 0.47 (ether); colorless liquid.

^{1}H NMR (300 MHz, $CDCl_3$): δ / ppm = 1.33, 1.39 (s, 6 H, CH_3(*Cby*)); 1.46 (m, 2 H, H-5); 1.48, 1.53 (s, 6 H, CH_3(*Cby*)); 1.81 (bs, 1 H, OH); 2.00-2.14 (m, 4 H, H-4, H-6); 3.69 (s, 2 H, CH_2(*Cby*)); 4.14 (m, 2 H, H-9); 4.60 (d, 2 H, H-1); 5.50-5.65 (m, 4 H, H-2, H-3, H-7, H-8).

$^3J_{1,2}$ = 5.1 Hz.

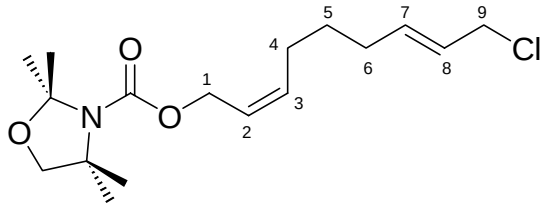
^{13}C NMR (75 MHz, $CDCl_3$): δ / ppm = 24.1, 25.2, 26.5 (CH_3(*Cby*)); 26.7, 28.6, 29.2, 31.3 (C-4, C-5, C-6); 59.7 (C(*Cby*)); 60.3 (C-9); 63.6 (C-1); 76.1, 76.3 (CH_2(*Cby*)); 94.9, 95.8 (C(*Cby*)); 124.4 (C-2); 129.9, 132.3 (C-7, C-8); 134.1 (C-3); 153.5 (C=O(*Cby*)).

IR (film): $\tilde{\nu}$ / cm^{-1} = 3451 (br), 2981, 2934, 2867, 1697, 1395, 1379, 1258, 1096, 1067, 733.

MS (70 eV): m/z (%) = 311 (0.5) [M^+], 296 (7) [$(M–CH_3)^+$], 294 (9) [$(M–H–H_2O)^+$], 156 (60) [*Cby*$^+$], 121 (16) [$(M–O$*Cby*$–H_2O)^+$], 114 (92), 79 (85), 67 (100), 59 (44) [$HOC(CH_3)_2^+$].

$C_{17}H_{29}NO_4$ (311.42)	calcd.	C 65.57	H 9.39	N 4.50
	found	C 65.92	H 9.72	N 4.67.

(2*Z*,7*E*)-9-Chloro-2,7-nonadienyl 2,2,4,4-tetramethyl-1,3-oxazolidine-3-carboxylate (3)



The carbamate **2** (550 mg, 1.78 mmol, 1.0 equiv.) and dry LiCl (75 mg, 1.78 mmol, 1.0 equiv.) were stirred in THF (5 ml) at –78°C. After injection of *n*-BuLi (1.2 ml, 1.96 mmol, 1.1 equiv., 1.6 M solution in hexane) and additional stirring for 15 min, CH_3SO_2Cl (245 mg, 2.14 mmol, 1.2 equiv.) was added and the reaction mixture was allowed to warm up to room temperature within 48 hrs. After addition of water (0.7 ml) and Et_2O (50 ml) the mixture was dried ($MgSO_4$), filtered and concentrated in vacuo. Flash-chromatography over silica gel(ether/pentane = 1:5) of the crude product furnished the allylic chloride **3** (411 mg) in 70% yield.

t_R = 19.17 min (HP1; 50°C, 10°C/min, 290°C, 10 min); R_f = 0.47 (ether/pentane = 2:5); colorless liquid.

^{1}H NMR (300 MHz, $CDCl_3$): δ / ppm = 1.34, 1.40 (s, 6 H, CH_3(*Cby*)); 1.44-1.59 (m, 8 H, H-5, CH_3(*Cby*)); 2.03-2.15 (m, 4 H, H-4, H-6); 3.70 (s, 2 H, CH_2(*Cby*)); 4.00 (dd, 2 H, H-9); 4.61 (d, 2 H, H-1); 5.52-5.64, 5.69-5.80 (m, 4 H, H-2, H-3, H-7, H-8).

$^3J_{1,2}$ = 5.1 Hz, $^4J_{7,9}$ = 0.9, $^3J_{8,9}$ = 6.9 Hz.

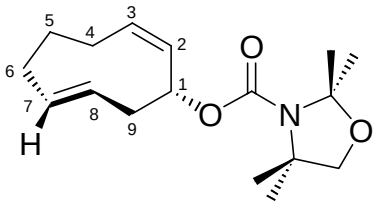
^{13}C NMR (75 MHz, $CDCl_3$): δ / ppm = 24.1, 25.3, 26.5 (CH_3(*Cby*)); 26.9, 28.5, 31.4 (C-4, C-5, C-6); 45.2 (C-9); 59.7, 60.6 (C(*Cby*)); 60.2 (C-1); 76.5, 76.6 (CH_2(*Cby*)); 95.8 (C(*Cby*)); 124.6 (C-8); 126.4 (C-2); 133.9 (C-7); 135.3 (C-3); 153.9 (C=O(*Cby*)).

IR (Film): $\tilde{\nu}$ / cm^{-1} = 2980, 2934, 2866, 1697, 1403, 1345, 1259, 1095, 1063, 967, 765.

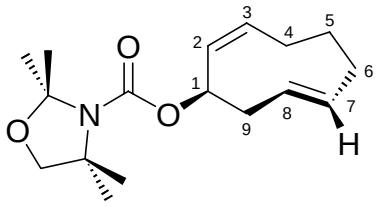
MS (70 eV): m/z (%) = 329 (0.3) [M^+], 314 (7) [$(M-CH_3)^+$], 294 (61) [$(M-Cl)^+$], 270 (11) [$(M+H-OC(CH_3)_2)^+$], 158 (26) [$(M+H-O$*Cby*$)^+$], 121 (42), 67 (100).

$C_{17}H_{28}ClNO_3$ (329.86)	calcd.	C 61.90	H 8.56	N 4.25
	found	C 62.08	H 8.79	N 4.41.

(1*R*,2*Z*,7*E*)-Cyclonona-2,7-dien-1-yl 2,2,4,4-tetramethyl-1,3-oxazolidine-3-carboxylate (5)



(*M*,*R*)-5



(*P*,*R*)-5

The allylic chloride **3** (150 mg, 0.45 mmol, 1.0 equiv.) and (–)-sparteine (213 mg, 0.91 mmol, 2.0 equiv.) were dissolved in toluene (5 ml) and cooled to –88°C. After dropwise injection of *n*-BuLi (0.57 ml, 0.91 mmol, 2.0 equiv., 1.6 M in hexane) the reaction mixture was stirred for 2 h. Addition of CH_3OH (0.4 ml), sat. NH_4Cl(aq) (0.2 ml) and Et_2O (35 ml) stopped the reaction and after warming up the solution to room temperature, drying ($MgSO_4$), filtration, evaporation of the solvent in vacuo, flash-chromatography over silica gel (ether/pentane = 1:5) furnished the slowly interconverting cyclononadienes (109 mg, 82%) **(*M*,*R*)-5** and **(*P*,*R*)-5** in a ratio of 7:3, when performing a rapid standard workup.

(*M*,*R*)-5 (unstable diastereomer):

R_f = 0.38 (ether/pentane = 2:5); colorless oil.

$[\alpha]_D^{20}$ = +15.0, $[\alpha]_{578}^{20}$ = +15.9, $[\alpha]_{546}^{20}$ = +18.3, $[\alpha]_{436}^{20}$ = +33.4, $[\alpha]_{365}^{20}$ = +57.9 (c = 1.200, $CHCl_3$), with 80% *ee*.

^{1}H NMR (600 MHz, $CDCl_3$): δ / ppm = 1.36-1.43 (m, 6 H, CH_3(*Cby*)); 1.48-1.60 (m, 7 H, H-5a, CH_3(*Cby*)); 1.74-1.82 (m, 1 H, H-9a); 1.83-1.92 (m, 1 H, H-6a); 1.92-2.00 (m, 3 H, H-4, H-5b); 2.40-2.43 (m, 1 H, H-6b); 2.61-2.64 (m, 1 H, H-9b); 3.71, 3.72 (s, 2 H, CH_2(*Cby*)); 5.24-5.28 (m, 1 H, H-2); 5.29-5.36 (m, 2 H, H-7, H-8); 5.44-5.53 (m, 2 H, H-1, H-3).

^{13}C NMR (150 MHz, $CDCl_3$): δ / ppm = 24.1, 25.2, 25.3, 25.5, 26.6, 26.7 (CH_3(*Cby*)); 28.3 (C-4); 32.1 (C-5); 34.1 (C-6); 34.6 (C-9); 74.9, 75.0 (C-1); 76.0, 76.6 (CH_2(*Cby*)); 123.4 (C-2); 124.2 (C-7); 136.9 (C-8); 137.8 (C-3); 151.7 (C=O(*Cby*)).

(*P*,*R*)-5 (stable diastereomer):

R_f = 0.43 (ether/pentane = 2:5); Mp. = 80.8 °C; white solid.

$[\alpha]_D^{20}$ = –58.2, $[\alpha]_{578}^{20}$ = –60.7, $[\alpha]_{546}^{20}$ = –69.7, $[\alpha]_{436}^{20}$ = –123.2, $[\alpha]_{365}^{20}$ = –203.4 (c = 0.555, $CHCl_3$), with 80% *ee*.

^{1}H NMR (600 MHz, $CDCl_3$): δ / ppm = 1.37, 1.40-1.47 (m, 7 H, H-5a, CH_3(*Cby*)); 1.52, 1.54, 1.55 (s, 6 H, CH_3(*Cby*)); 1.61-1.68 (m, 1 H, H-4a); 1.75-1.90 (m, 2 H, H-6a, H-9a); 1.91-1.98 (m, 2 H, H-4b, H-5b); 2.35-2.40 (m, 1 H, H-6b); 2.57-2.62 (m, 1 H, H-9b); 3.70, 3.71 (s, 2 H, CH_2(*Cby*)); 5.00-5.06 (m, 1 H, H-2); 5.08-5.12 (m, 1 H, H-1); 5.21 (ddd, 1 H, H-8); 5.25-5.31 (m, 1 H, H-7); 5.34 (ddd, 1 H, H-3).

$^3J_{2,3}$ = $^3J_{3,4a}$ = 11.4 Hz, $^3J_{3,4b}$ = 3.7 Hz, $^3J_{7,8}$ = 15.0 Hz, $^3J_{8,9a}$ = 10.8 Hz, $^3J_{8,9b}$ = 4.8 Hz.
The coupling constants $^3J_{2,3}$ = 11.4 Hz and $^3J_{7,8}$ = 15.0 Hz are typical for a *Z* and an *E* double bond.

^{13}C NMR (150 MHz, $CDCl_3$): δ / ppm = 24.1, 24.2, 25.3, 25.4, 25.5, 25.6 (CH_3(*Cby*)); 27.4 (C-4); 30.4 (C-5); 34.1 (C-6); 37.4 (C-9); 59.7, 60.6 (C(*Cby*)); 73.0 (C-1); 76.0, 76.3 (CH_2(*Cby*)); 124.7, 124.8 (C-2); 125.2 (C-8); 134.1, 134.2 (C-3); 137.0 (C-7); 151.5, 152.2 (C=O(*Cby*)).
Eine C(*Cby*)-Gruppe ist nicht zu erkennen.

IR (KBr): $\tilde{\nu}$ / cm^{-1} = 2985, 2933, 2859, 1692, 1445, 1392, 1366, 1256, 1098, 1066, 767, 760.

MS (70 eV): m/z (%) = 293 (3) [M^+], 278 (2) [$(M–CH_3)^+$], 156 (56) [Cby^+], 121 (16) [$(M–OCby)^+$], 39 (40) [$(Cby–OC(CH_3)_2)^+$], 59 (100) [$HOC(CH_3)_2^+$].

$C_{17}H_{27}NO_3$ (293.40)	calcd.	C 69.59	H 9.28	N 4.77
	found	C 69.35	H 9.42	N 4.39.

2. Information about the X-ray analysis

X-ray crystal structure analysis of **HOP1345**: formula $C_{17}H_{27}NO_3$, *M* = 293.40, colorless crystal 0.30 x 0.15 x 0.05 mm, *a* = 7.295(2), *b* = 10.900(2), *c* = 11.266(2) Å, α = 76.21(2), β = 88.53(2), γ = 76.68(2)°, *V* = 853.7(3) $Å^3$, ρ_{calc} = 1.141 g cm^{-3}, μ = 6.16 cm^{-1}, empirical absorption correction via ψ scan data (0.837 ≤ *T* ≤ 0.970), *Z* = 2, triclinic, space group *P*1bar (No. 2), λ = 1.54178 Å, *T* = 223 K, ω/2θ scans, 3752 reflections collected (-*h*, ±*k*, ±*l*), [(sinθ)/λ] = 0.62 $Å^{-1}$, 3466 (R_{int} = 0.023) and 1642 observed reflections [$I \geq 2\ \sigma(I)$], 225 refined parameters, *R* = 0.063, wR^2 = 0.162, max. residual electron density 0.22 (-0.20) e $Å^{-3}$, disorder in the groups C3-C4-C5 (0.73(1)/0.27), C6-C7-C8 (0.69(1)/0.31), and O15 (0.87(1)/0.13) is refined with splitted positions, hydrogens calculated and refined as riding atoms.

Data set was collected with an Enraf-Nonius CAD4 diffractometer. Programs used: data collection EXPRESS (Nonius B.V., 1994) , data reduction MolEN (K. Fair, Enraf-Nonius B.V., 1990), structure solution SHELXS-97 (G.M. Sheldrick, *Acta Cryst.* **1990**, *A46*, 467-473), structure refinement SHELXL-97 (G.M. Sheldrick, Universität Göttingen, 1997).

3. Ab inition DFT calculations

Table: Cartesian coordinates, HF-energies, gradient norm (RMSD) (B3LYP/6-31G(d)) for all stationary points reported in Table 2, taken from the Gaussian98 archive entry.

Table (continued)

$(P,R)_{eq}$-**5'**

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$(P,R)_{ax}$-**5'**

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C 2.2924322975 -0.62491052 -0.2947956549
C 2.2041100833 0.6983843119 -0.1415351359
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Table (continued)

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H -1.7893284628 2.2057701583 2.9245529591
H -0.5418727203 1.7451067346 1.7441213381
H -1.9120419936 2.7645669775 1.2420991946

Version=x86-Linux-G98RevA.7
HF=-673.8864096
RMSD=6.213e-09
RMSF=3.427e-06
PG=C01 [X(C12H19N1O2)]
```

Table (continued)

$(M,R)_{eq}$-**5'**

```
C 0.5127542877 -0.245705471 -1.6272216391
C 0.1668549126 -0.1772463689 -0.1620532059
C 1.415875429 -0.0370553884 0.7604248351
C 2.2121032887 1.1315199692 0.2441420541
C 1.7642988876 2.3882162068 0.309550448
C 2.1615984248 3.4686820107 -0.6689517573
C 1.7801604172 3.0715542579 -2.1283574237
C 0.447027024 2.2635987635 -2.2714704939
C 0.6493570795 0.7772721684 -2.4826914441
H 0.728928366 -1.2510883587 -1.987864929
O -0.5461365646 -1.4011207106 0.1478509421
H -0.4964389089 0.6616687138 0.0557648243
H 1.9901927684 -0.9697396207 0.7359807552
H 1.0543760008 0.1174524816 1.7825240731
H 3.0354037237 0.8991446928 -0.4313466391
H 0.913965927 2.6019396126 0.9593156714
H 3.2385930162 3.6802652561 -0.631216613
H 1.6555030342 4.4040561313 -0.4028335807
H 2.5951138574 2.4763098656 -2.5580065137
H 1.7222263353 3.9849321647 -2.7335350575
H -0.0940634596 2.6459710306 -3.1470480223
H -0.1978626063 2.4507157662 -1.406849025
H 0.9756985078 0.518326953 -3.4919096431
C -1.411503943 -1.33903102 1.1983682691
O -1.6127783235 -0.3252759477 1.8518851678
N -2.0164875955 -2.5444040689 1.4289975847
C -1.813093869 -3.734359515 0.6196152305
C -2.9999813794 -2.6419560078 2.4938277802
H -2.7325153819 -3.9999727071 0.0785138235
H -1.0159241921 -3.5651968419 -0.1001362592
H -1.541183271 -4.582332392 1.2621614449
H -3.9937124853 -2.8748859351 2.0863944213
H -2.7225326255 -3.4383912264 3.1969938731
H -3.0417396899 -1.6901114706 3.0211295059

Version=x86-Linux-G98RevA.7
HF=-673.8811558
RMSD=6.482e-09
RMSF=3.925e-06
PG=C01 [X(C12H19N1O2)]
```

Table (continued)

$(P,R)_{ax\text{-}eq}$-**TS5'**

```
C 0.6948621512 1.3347995636 -0.4120435358
C -0.0449944585 0.015902523 -0.2318915998
C 0.4315992227 -1.0768198589 0.7462183212
C 1.7815024912 -1.5290542261 0.2948131986
C 2.909163961 -1.2021071374 0.9245083188
C 4.2141224198 -1.026788036 0.1959957345
C 4.0473097338 0.2288001312 -0.7016357252
C 3.3591710381 1.4341089588 0.0168277822
C 1.9393785494 1.8514027935 -0.3691046247
H -0.0441212163 2.0598406235 -0.7552638253
H -0.145415611 -0.4494347041 -1.220363813
O -1.3878448235 0.4203604289 0.1690406789
H 0.4684380604 -0.6734950068 1.7645441095
H -0.3212561449 -1.8736191469 0.7124271256
H 1.834927302 -1.9356596208 -0.7180832053
H 2.8384964193 -0.7753285672 1.9254134041
H 5.0446123777 -0.8874874209 0.8986485231
H 4.4614751553 -1.894599571 -0.4281979744
H 5.029902687 0.5464258788 -1.0736491007
H 3.4559317636 -0.0486780904 -1.5809339085
H 3.4058867621 1.2881221828 1.1027388398
H 3.9761959634 2.3201428352 -0.1685395729
H 1.9293344181 2.900336872 -0.6703037269
C -2.4153406835 -0.3190834843 -0.3367478178
O -2.261899561 -1.2570746725 -1.1059878158
N -3.6264925224 0.1153663222 0.1275249382
C -3.8049173153 1.2648220102 0.9995914312
C -4.834818042 -0.5262969549 -0.3619115699
H -5.4448783979 -0.8802569989 0.4794260433
H -5.4388227598 0.177224584 -0.9519928453
H -4.5540234193 -1.3715397555 -0.9883878024
H -4.4421441783 0.9901541773 1.8502435255
H -2.8415724163 1.6033602271 1.3735509264
H -4.2917984396 2.0925234982 0.4639063256

Version=x86-Linux-G98RevA.7
HF=-673.8645074
RMSD=7.056e-09
RMSF=2.253e-06
PG=C01 [X(C12H19N1O2)]
```

Table (continued)

$(M\text{-}P,R)_{ax}$-**TS5'**

```
C 0.1938433825 -1.5786309623 -1.6206531647
C 0.2155930468 -1.5181345 -0.0877507672
C 1.5910181329 -1.498794643 0.6728645667
C 2.4442332856 -0.2412215794 0.5017919009
C 2.1543298118 0.4831875294 -0.5752977915
C 2.406211707 1.7436518785 -1.3477821901
C 1.6137490829 1.5789224267 -2.6857434375
C 0.1987818198 0.8962434523 -2.5368773012
C 0.1679903976 -0.6357532269 -2.5856400723
H 0.1968274066 -2.6097712148 -1.9748828464
H -0.2909706484 -2.4211672758 0.2615932953
O -0.5896159405 -0.3963801017 0.3588671647
H 2.150069056 -2.4010875289 0.3793613233
H 1.3360179914 -1.6451501896 1.7300434814
H 3.1970803444 -0.0171925563 1.2582879865
H 1.3998201802 -0.0293886527 -1.1060250205
H 3.4646939223 1.957062672 -1.5470719009
H 2.0165421814 2.6139254465 -0.7986597122
H 2.2138052404 0.9852869238 -3.3876923373
H 1.4736380265 2.5608104609 -3.1526665572
H -0.4175250549 1.2488427716 -3.3733888731
H -0.2821594952 1.2585677439 -1.6230413748
H 0.1526513183 -1.0290628962 -3.6035301637
C -1.3554725706 -0.6196200601 1.4653128717
O -1.4630448557 -1.7076842256 2.0123543332
N -1.9777157972 0.5248275329 1.8838267558
C -1.8610092059 1.8006954742 1.1962045637
C -2.9681447515 0.4307523908 2.9440022619
H -2.7619653621 1.1780851997 3.7203615
H -3.9816170602 0.6072393762 2.5560197017
H -2.9206694534 -0.5667959061 3.378185173
H -1.9181363421 2.6070745176 1.9360971441
H -0.9020242983 1.8631349564 0.6846257279
H -2.6675258369 1.9505189583 0.4632355368

Version=Sun-SVR4-Unix-G98RevA.7
HF=-673.8421314
RMSD=7.210e-09
RMSF=1.808e-06
PG=C01 [X(C12H19N1O2)]
```

Table (continued)

$(M,R)_{ax\text{-}eq}$-**TS5'**

```
H 1.1388963884 -0.6013760007 -2.5003220329
C 1.1506217878 -0.8406403812 -1.4355348439
C 2.4127305975 -0.9778928769 -0.9766969306
C 3.1907017181 -1.2957958362 0.3018522136
C 2.8776201387 -0.599685808 1.6601922658
C 2.1273019257 -1.5020140333 2.6734110062
C 0.989594627 -2.1301119358 1.91670396
C -0.0265846489 -1.4027953807 1.4544037655
C -0.7718345582 -1.7450599662 0.2091112945
C -0.2944110451 -0.8445869358 -0.9483278244
O -0.5989843829 0.5502769183 -0.6279553148
H -0.9119911993 -1.0991733434 -1.8134788713
H -0.5950506595 -2.7894097754 -0.077106656
H -1.85609715 -1.5986971173 0.2866487052
H -0.1751077456 -0.3920092342 1.8363288579
H 1.1522272602 -3.1261400409 1.5034828196
H 2.8057263694 -2.2610583977 3.0819212659
H 1.777753169 -0.8937578633 3.5174446718
H 3.8225220559 -0.2592804179 2.1043153564
H 2.2759301054 0.2969115558 1.4759895728
H 3.1878712793 -2.3860501539 0.4424462499
H 4.2317646099 -1.0593463544 0.0536772638
H 3.1250221193 -0.8573647817 -1.7959304569
C -1.8344578152 0.9964190274 -0.9951484204
O -2.6817338117 0.2925814468 -1.5259743277
N -2.0012065818 2.3213753365 -0.6973506788
C -0.9881121073 3.1571905975 -0.0746109687
C -3.2836239315 2.9461236633 -0.9729054584
H -3.7467643672 3.3069864736 -0.0440677772
H -3.1553850357 3.803173493 -1.6475455077
H -3.9377739084 2.2121586778 -1.4410626436
H -1.3082624111 3.4770807878 0.9272944863
H -0.0520836206 2.609989726 0.0087098221
H -0.8222857619 4.0579676857 -0.6805535898

Version=Sun-SVR4-Unix-G98RevA.7
HF=-673.861961
RMSD=3.978e-09
RMSF=3.381e-06
PG=C01 [X(C12H19N1O2)]
```

Table (continued)

$(M\text{-}P,R)_{eq}$-**TS5'**

```
C 3.3151018803 -0.863060671 -2.3638871189
N 3.2761067138 -0.6948400031 -0.9207960615
C 4.5341741329 -0.8569131334 -0.2121614065
C 2.1749418298 -0.2822516633 -0.2200713334
O 2.1490568247 -0.0987180029 0.9864790736
O 1.1005330766 -0.095598239 -1.0426935588
C -0.1545344762 0.2489598662 -0.3972171731
C -0.7780924748 1.3680605927 -1.2986957716
C -1.9538398538 2.1014979402 -0.6535708098
C -2.5501543486 1.4295256286 0.3290443968
C -3.5822212147 1.433128919 1.4172296038
C -3.6454655519 -0.0427021531 1.9317881485
C -2.250718199 -0.7766253603 2.0298096254
C -1.7418265732 -1.4814662844 0.7663175299
C -0.9161178696 -1.0679558199 -0.2163101652
H -0.726853329 -1.7683709775 -1.0298576028
H 0.084294254 0.6848705416 0.574611733
H -1.0548426905 0.9459710068 -2.2764729237
H 0.0401218853 2.071606276 -1.4987575214
H -2.2075718452 3.0993318264 -1.011934536
H -2.0872459682 0.4833183779 0.3925119092
H -4.576103813 1.7822451081 1.1081830273
H -3.265981584 2.0923139134 2.2392437417
H -4.2969903098 -0.6264467734 1.2686337552
H -4.1129150266 -0.0641941741 2.9228951014
H -2.3502815373 -1.5520738575 2.7991090498
H -1.499432727 -0.0717203564 2.4075829313
H -2.1510294304 -2.4844191484 0.6371108078
H 3.7586056051 -1.8362312022 -2.6115970121
H 2.3085700529 -0.818343552 -2.7728040094
H 3.9274668235 -0.0811593357 -2.8363577056
H 4.9455636311 -1.8583582248 -0.3938625835
H 5.2723689059 -0.1159542654 -0.5504353186
H 4.3553072087 -0.7251623922 0.8538323135

Version=x86-Linux-G98RevA.7
HF=-673.8459285
RMSD=3.886e-09
RMSF=1.938e-06
PG=C01 [X(C12H19N1O2)]
```