Conformational Dynamics In Nitrogen-Fused Azabicycles

Anatoly M. Belostotskii* and Elena Markevich

Chemistry Department, Bar-Ilan University, Ramat-Gan 52900, Israel

SUPPORTING INFORMATION

Content

1.	Conformers of 1a	S1-S5
2.	Conformers of 1b	S6-S10
3.	Conformations of 3	S11-S29
4.	Conformations of 4	S30-S50
5.	Conformers of 5	S51-S66
6.	Conformations of 6	S68-S122
7.	Conformations of 7a	S123-S138
8.	Conformations of 8	S139-S162

Isosparteine **1a** (energy minimum 1)

Item	Value	Threshold	Converged?
Maximum Force	0.000250	0.000450	YES
RMS Force	0.000044	0.000300	YES
Maximum Displacement	0.000159	0.001800	YES
RMS Displacement	0.000047	0.001200	YES

Predicted change in Energy=-1.996752D-08
Optimization completed.

-- Stationary point found.

! Optimized Parameters !
! (Angstroms and Degrees) !

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.718836	0.661751	-0.384224
2	6	0	0.631950	1.531372	-1.040573
3	6	0	-0.000039	2.447663	0.001048
4	6	0	-0.632035	1.530451	1.041892
5	6	0	0.494129	0.756484	1.721488
6	7	0	1.225931	-0.083141	0.781327
7	6	0	-0.494339	0.758196	-1.720880
8	6	0	-1.718870	0.661433	0.384843
9	7	0	-1.226059	-0.082340	-0.781488
10	6	0	-2.331391	-0.746371	-1.468451
11	6	0	-2.343630	-0.327361	1.366562
12	6	0	-3.005131	-1.765501	-0.559955
13	6	0	-3.495119	-1.090832	0.717620

S2

14	6	0	2.331219	-0.747790	1.467733
15	6	0	2.343909	-0.326052	-1.366774
16	6	0	3.495411	-1.089916	-0.718412
17	6	0	3.005197	-1.765958	0.558326
18	1	0	1.136397	2.129217	-1.814474
19	1	0	0.753103	3.096741	0.467706
20	1	0	-0.753163	3.097172	-0.465063
21	1	0	-1.136457	2.127646	1.816334
22	1	0	1.161519	1.496969	2.214783
23	1	0	0.105785	0.109868	2.517062
24	1	0	-1.161784	1.499183	-2.213367
25	1	0	-0.106117	0.112374	-2.517137
26	1	0	-2.518313	1.369363	0.060150
27	1	0	-3.083217	-0.009277	-1.823723
28	1	0	-1.924158	-1.242878	-2.357775
29	1	0	-1.567536	-1.036774	1.674302
30	1	0	-2.685442	0.211221	2.260614
31	1	0	-3.834240	-2.246618	-1.093528
32	1	0	-2.275278	-2.544162	-0.309988
33	1	0	-3.912138	-1.828999	1.413175
34	1	0	-4.305312	-0.390423	0.472720
35	1	0	3.082978	-0.011041	1.823860
36	1	0	1.923871	-1.245219	2.356483
37	1	0	2.518188	1.369398	-0.058675
38	1	0	2.685779	0.213391	-2.260279
39	1	0	1.568038	-1.035371	-1.675267
40	1	0	3.912705	-1.827297	-1.414635
41	1	0	4.305417	-0.389598	-0.472618
42	1	0	2.275431	-2.544402	0.307438
43	1	0	3.834254	-2.247541	1.091556

Rotational constants (GHZ): 0.7784443 0.3664237 0.3562292
 Isotopes: C-12,C-12,C-12,C-12,N-14,C-12,C-12,N-14,C-12,C-12,C-12,C-12,
 C-12,C-12,C-12,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,
 -1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1

Dipole moment (Debye):

X= 0.0001 Y= 0.7032 Z= 0.0003 Tot= 0.7032

Quadrupole moment (Debye-Ang):

XX= -106.5432 YY= -107.2405 ZZ= -105.4398

XY= -0.0004 XZ= -0.1444 YZ= -0.0008

Octapole moment (Debye-Ang**2):

XXX= 0.0039 YYY= -2.8977 ZZZ= -0.0058 XYY= 0.0018

XXY= -2.1350 XXZ= -0.0033 XZZ= -0.0034 YZZ= -2.6499

YYZ= 0.0007 XYZ= -2.5602

Hexadecapole moment (Debye-Ang**3):

XXXX= -3251.7842 YYYY= -1152.1373 ZZZZ= -1032.0593 XXXY= -0.0104

XXXZ= 14.1695 YYYY= -0.0009 YYYZ= -0.0147 ZZZX= -3.8201

ZZZY= 0.0083 XXYY= -723.1052 XXZZ= -710.8087 YYZZ= -355.9428

XXYZ= 0.0068 YYXZ= -0.6993 ZZXZ= 0.0004

N-N= 1.399590814321D+03 E-N=-4.411827518533D+03 KE= 6.913039486074D+02

1\1\GINC-ILANIT\FOpt\RMP2-FC\6-31G(d)\C15H26N2\BELOSTOT\26-May-2002\1\
 \# MP2/6-31G* GEOM=ALLCHECKPOINT GUESS=CHECKPOINT OPT=Z-MATRIX\alpha

isosparteine, the lowest energy conformer\0,1\C\1,r2\C,2,r3,1,a3\C,
 3,r4,2,a4,1,d4,0\C,4,r5,3,a5,2,d5,0\N,5,r6,4,a6,3,d6,0\C,2,r7,1,a7,3,d
 7,0\C,4,r8,3,a8,2,d8,0\N,7,r9,2,a9,1,d9,0\C,9,r10,7,a10,2,d10,0\C,8,r1
 1,4,a11,3,d11,0\C,10,r12,9,a12,7,d12,0\C,12,r13,10,a13,9,d13,0\C,6,r14
 ,5,a14,4,d14,0\C,1,r15,2,a15,3,d15,0\C,15,r16,1,a16,2,d16,0\C,16,r17,1
 5,a17,1,d17,0\H,2,r18,1,a18,3,d18,0\H,3,r19,2,a19,1,d19,0\H,3,r20,2,a2
 0,1,d20,0\H,4,r21,3,a21,2,d21,0\H,5,r22,4,a22,3,d22,0\H,5,r23,4,a23,3,
 d23,0\H,7,r24,2,a24,1,d24,0\H,7,r25,2,a25,1,d25,0\H,8,r26,4,a26,3,d26,
 0\H,10,r27,9,a27,7,d27,0\H,10,r28,9,a28,7,d28,0\H,11,r29,8,a29,4,d29,0
 \H,11,r30,8,a30,4,d30,0\H,12,r31,10,a31,9,d31,0\H,12,r32,10,a32,9,d32,
 0\H,13,r33,12,a33,10,d33,0\H,13,r34,12,a34,10,d34,0\H,14,r35,6,a35,5,d
 35,0\H,14,r36,6,a36,5,d36,0\H,1,r37,2,a37,3,d37,0\H,15,r38,1,a38,2,d38
 ,0\H,15,r39,1,a39,2,d39,0\H,16,r40,15,a40,1,d40,0\H,16,r41,15,a41,1,d4
 1,0\H,17,r42,16,a42,15,d42,0\H,17,r43,16,a43,15,d43,0\H,r2=1.53894623\H
 3=1.52445886\H,a3=109.93917142\H,r4=1.52448419\H,a4=106.06572443\H,d4=298.6241
 1669\H,r5=1.5261455\H,a5=107.65234506\H,d5=64.76503682\H,r6=1.45753541\H,a6=112.
 04897375\H,d6=298.08419639\H,r7=1.5261537\H,a7=115.15368819\H,d7=238.22387663\

r8=1.53886836\ a8=109.93998631\ d8=298.62388973\ r9=1.45752236\ a9=112.046
 12704\ d9=61.0791831\ r10=1.46103208\ a10=109.80772863\ d10=177.16712988\ r
 11=1.52702613\ a11=112.34145812\ d11=177.27524882\ r12=1.52247027\ a12=111
 .00528628\ d12=172.76636636\ r13=1.52560279\ a13=110.23163344\ d13=57.1060
 4783\ r14=1.46101826\ a14=109.80683403\ d14=177.15983371\ r15=1.52704773\ a
 15=112.34643186\ d15=177.28745149\ r16=1.52637478\ a16=111.05190181\ d16=1
 75.22636792\ r17=1.52558246\ a17=109.56276455\ d17=55.06029298\ r18=1.1003
 673\ a18=106.45124508\ d18=119.25666396\ r19=1.09831481\ a19=111.17674656\
 d19=58.74923535\ r20=1.09832447\ a20=110.47167569\ d20=178.03906655\ r21=1
 .10038318\ a21=110.12246846\ d21=181.63652428\ r22=1.11223494\ a22=107.616
 59505\ d22=61.14691029\ r23=1.09629418\ a23=111.15423546\ d23=177.35800069
 \ r24=1.11224468\ a24=107.62141727\ d24=184.14214425\ r25=1.09627882\ a25=1
 11.15418031\ d25=300.35501622\ r26=1.11610992\ a26=105.77727231\ d26=294.5
 613144\ r27=1.11120152\ a27=111.14411944\ d27=295.02296211\ r28=1.09692942
 \ a28=107.82176052\ d28=51.98752819\ r29=1.09557872\ a29=108.06220373\ d29=
 295.05721669\ r30=1.09828703\ a30=109.45942001\ d30=52.46468666\ r31=1.097
 08551\ a31=109.74123708\ d31=179.66642778\ r32=1.09612162\ a32=108.4781425
 \ d32=296.98137897\ r33=1.09662702\ a33=110.83071039\ d33=184.40878499\ r34
 =1.09861796\ a34=109.39746546\ d34=66.8262107\ r35=1.11120056\ a35=111.146
 46263\ d35=295.02821604\ r36=1.09692541\ a36=107.81902788\ d36=51.99327925
 \ r37=1.11611329\ a37=105.77971276\ d37=294.57455847\ r38=1.09828263\ a38=1
 09.46041128\ d38=52.46126493\ r39=1.0955725\ a39=108.06553502\ d39=295.049
 74734\ r40=1.0966275\ a40=110.72560069\ d40=177.60656408\ r41=1.09862118\ a
 41=109.40487552\ d41=295.13246363\ r42=1.09611953\ a42=109.69952767\ d42=6
 6.2737794\ r43=1.09708268\ a43=111.00559267\ d43=185.07650373\ \\Version=SG
 I64-G98RevA.7\HF=-692.0558392\MP2=-694.3546939\RMSE=3.243e-09\RMSE=5.5
 72e-06\Dipole=0.0874481,0.1411196,0.1136164\PG=C01 [X(C15H26N2)]\ \@

Dipole moment (Debye):
X= -0.1130 Y= 0.6962 Z= -0.0391 Tot= 0.7064

Quadrupole moment (Debye-Ang):

XX= -106.8744 YY= -107.5323 ZZ= -105.5010

XY= 0.2748 XZ= -0.1921 YZ= 0.1451

Octapole moment (Debye-Ang**2):

XXX= 1.2636 YYY= -0.8733 ZZZ= 1.7618 XYY= -2.0706

XXY= -1.1304 XXZ= -0.4894 XZZ= 0.1657 YZZ= -2.1151

YYZ= 0.6148 XYZ= -1.8221

Hexadecapole moment (Debye-Ang**3):

XXXX= -2797.1756 YYYY= -1295.0392 ZZZZ= -1012.1491 XXXY= 1.7372

XXXZ= 8.9901 YYYY= 4.7591 YYYZ= 2.8108 ZZZX= -3.5537

ZZZY= -1.1715 XXYX= -678.0548 XXZZ= -639.6613 YYZZ= -378.8118

XXYZ= 2.2779 YYXZ= -1.0929 ZZXY= 0.7436

N-N= 1.415155962751D+03 E-N=-4.443025112865D+03 KE= 6.912872432261D+02

1\1\GINC-ILANIT\FOpt\RMP2-FC\6-31G(d)\C15H26N2\APED\19-May-2002\1\# M
P2/6-31G* OPT=Z-MATRIX GEOM=CHECKPOINT GUESS=CHECKPOINT\alpha isospar

teine, the second in energy conformer\0,1\1C,1,r2\1C,2,r3,1,a3\1C,3,r4
,2,a4,1,d4,0\1C,4,r5,3,a5,2,d5,0\1N,5,r6,4,a6,3,d6,0\1C,2,r7,1,a7,3,d7,0\1
C,4,r8,3,a8,2,d8,0\1N,7,r9,2,a9,1,d9,0\1C,9,r10,7,a10,2,d10,0\1C,8,r11,4,
a11,3,d11,0\1C,10,r12,9,a12,7,d12,0\1C,12,r13,10,a13,9,d13,0\1C,6,r14,5,a
14,4,d14,0\1C,1,r15,2,a15,3,d15,0\1C,15,r16,1,a16,2,d16,0\1C,16,r17,15,a1
7,1,d17,0\1H,2,r18,1,a18,3,d18,0\1H,3,r19,2,a19,1,d19,0\1H,3,r20,2,a20,1,
d20,0\1H,4,r21,3,a21,2,d21,0\1H,5,r22,4,a22,3,d22,0\1H,5,r23,4,a23,3,d23,
0\1H,7,r24,2,a24,1,d24,0\1H,7,r25,2,a25,1,d25,0\1H,8,r26,4,a26,3,d26,0\1H,
10,r27,9,a27,7,d27,0\1H,10,r28,9,a28,7,d28,0\1H,11,r29,8,a29,4,d29,0\1H,1
1,r30,8,a30,4,d30,0\1H,12,r31,10,a31,9,d31,0\1H,12,r32,10,a32,9,d32,0\1H,
13,r33,12,a33,10,d33,0\1H,13,r34,12,a34,10,d34,0\1H,14,r35,6,a35,5,d35,0
\1H,14,r36,6,a36,5,d36,0\1H,1,r37,2,a37,3,d37,0\1H,15,r38,1,a38,2,d38,0\1H
,15,r39,1,a39,2,d39,0\1H,16,r40,15,a40,1,d40,0\1H,16,r41,15,a41,1,d41,0\1
H,17,r42,16,a42,15,d42,0\1H,17,r43,16,a43,15,d43,0\1H,17,r44,16,a44,15,d44,0\1H,17,r45,16,a45,15,d45,0\1H,17,r46,16,a46,15,d46,0\1H,17,r47,16,a47,15,d47,0\1H,17,r48,16,a48,15,d48,0\1H,17,r49,16,a49,15,d49,0\1H,17,r50,16,a50,15,d50,0\1H,17,r51,16,a51,15,d51,0\1H,17,r52,16,a52,15,d52,0\1H,17,r53,16,a53,15,d53,0\1H,17,r54,16,a54,15,d54,0\1H,17,r55,16,a55,15,d55,0\1H,17,r56,16,a56,15,d56,0\1H,17,r57,16,a57,15,d57,0\1H,17,r58,16,a58,15,d58,0\1H,17,r59,16,a59,15,d59,0\1H,17,r60,16,a60,15,d60,0\1H,17,r61,16,a61,15,d61,0\1H,17,r62,16,a62,15,d62,0\1H,17,r63,16,a63,15,d63,0\1H,17,r64,16,a64,15,d64,0\1H,17,r65,16,a65,15,d65,0\1H,17,r66,16,a66,15,d66,0\1H,17,r67,16,a67,15,d67,0\1H,17,r68,16,a68,15,d68,0\1H,17,r69,16,a69,15,d69,0\1H,17,r70,16,a70,15,d70,0\1H,17,r71,16,a71,15,d71,0\1H,17,r72,16,a72,15,d72,0\1H,17,r73,16,a73,15,d73,0\1H,17,r74,16,a74,15,d74,0\1H,17,r75,16,a75,15,d75,0\1H,17,r76,16,a76,15,d76,0\1H,17,r77,16,a77,15,d77,0\1H,17,r78,16,a78,15,d78,0\1H,17,r79,16,a79,15,d79,0\1H,17,r80,16,a80,15,d80,0\1H,17,r81,16,a81,15,d81,0\1H,17,r82,16,a82,15,d82,0\1H,17,r83,16,a83,15,d83,0\1H,17,r84,16,a84,15,d84,0\1H,17,r85,16,a85,15,d85,0\1H,17,r86,16,a86,15,d86,0\1H,17,r87,16,a87,15,d87,0\1H,17,r88,16,a88,15,d88,0\1H,17,r89,16,a89,15,d89,0\1H,17,r90,16,a90,15,d90,0\1H,17,r91,16,a91,15,d91,0\1H,17,r92,16,a92,15,d92,0\1H,17,r93,16,a93,15,d93,0\1H,17,r94,16,a94,15,d94,0\1H,17,r95,16,a95,15,d95,0\1H,17,r96,16,a96,15,d96,0\1H,17,r97,16,a97,15,d97,0\1H,17,r98,16,a98,15,d98,0\1H,17,r99,16,a99,15,d99,0\1H,17,r100,16,a100,15,d100,0\1H,17,r101,16,a101,15,d101,0\1H,17,r102,16,a102,15,d102,0\1H,17,r103,16,a103,15,d103,0\1H,17,r104,16,a104,15,d104,0\1H,17,r105,16,a105,15,d105,0\1H,17,r106,16,a106,15,d106,0\1H,17,r107,16,a107,15,d107,0\1H,17,r108,16,a108,15,d108,0\1H,17,r109,16,a109,15,d109,0\1H,17,r110,16,a110,15,d110,0\1H,17,r111,16,a111,15,d111,0\1H,17,r112,16,a112,15,d112,0\1H,17,r113,16,a113,15,d113,0\1H,17,r114,16,a114,15,d114,0\1H,17,r115,16,a115,15,d115,0\1H,17,r116,16,a116,15,d116,0\1H,17,r117,16,a117,15,d117,0\1H,17,r118,16,a118,15,d118,0\1H,17,r119,16,a119,15,d119,0\1H,17,r120,16,a120,15,d120,0\1H,17,r121,16,a121,15,d121,0\1H,17,r122,16,a122,15,d122,0\1H,17,r123,16,a123,15,d123,0\1H,17,r124,16,a124,15,d124,0\1H,17,r125,16,a125,15,d125,0\1H,17,r126,16,a126,15,d126,0\1H,17,r127,16,a127,15,d127,0\1H,17,r128,16,a128,15,d128,0\1H,17,r129,16,a129,15,d129,0\1H,17,r130,16,a130,15,d130,0\1H,17,r131,16,a131,15,d131,0\1H,17,r132,16,a132,15,d132,0\1H,17,r133,16,a133,15,d133,0\1H,17,r134,16,a134,15,d134,0\1H,17,r135,16,a135,15,d135,0\1H,17,r136,16,a136,15,d136,0\1H,17,r137,16,a137,15,d137,0\1H,17,r138,16,a138,15,d138,0\1H,17,r139,16,a139,15,d139,0\1H,17,r140,16,a140,15,d140,0\1H,17,r141,16,a141,15,d141,0\1H,17,r142,16,a142,15,d142,0\1H,17,r143,16,a143,15,d143,0\1H,17,r144,16,a144,15,d144,0\1H,17,r145,16,a145,15,d145,0\1H,17,r146,16,a146,15,d146,0\1H,17,r147,16,a147,15,d147,0\1H,17,r148,16,a148,15,d148,0\1H,17,r149,16,a149,15,d149,0\1H,17,r150,16,a150,15,d150,0\1H,17,r151,16,a151,15,d151,0\1H,17,r152,16,a152,15,d152,0\1H,17,r153,16,a153,15,d153,0\1H,17,r154,16,a154,15,d154,0\1H,17,r155,16,a155,15,d155,0\1H,17,r156,16,a156,15,d156,0\1H,17,r157,16,a157,15,d157,0\1H,17,r158,16,a158,15,d158,0\1H,17,r159,16,a159,15,d159,0\1H,17,r160,16,a160,15,d160,0\1H,17,r161,16,a161,15,d161,0\1H,17,r162,16,a162,15,d162,0\1H,17,r163,16,a163,15,d163,0\1H,17,r164,16,a164,15,d164,0\1H,17,r165,16,a165,15,d165,0\1H,17,r166,16,a166,15,d166,0\1H,17,r167,16,a167,15,d167,0\1H,17,r168,16,a168,15,d168,0\1H,17,r169,16,a169,15,d169,0\1H,17,r170,16,a170,15,d170,0\1H,17,r171,16,a171,15,d171,0\1H,17,r172,16,a172,15,d172,0\1H,17,r173,16,a173,15,d173,0\1H,17,r174,16,a174,15,d174,0\1H,17,r175,16,a175,15,d175,0\1H,17,r176,16,a176,15,d176,0\1H,17,r177,16,a177,15,d177,0\1H,17,r178,16,a178,15,d178,0\1H,17,r179,16,a179,15,d179,0\1H,17,r180,16,a180,15,d180,0\1H,17,r181,16,a181,15,d181,0\1H,17,r182,16,a182,15,d182,0\1H,17,r183,16,a183,15,d183,0\1H,17,r184,16,a184,15,d184,0\1H,17,r185,16,a185,15,d185,0\1H,17,r186,16,a186,15,d186,0\1H,17,r187,16,a187,15,d187,0\1H,17,r188,16,a188,15,d188,0\1H,17,r189,16,a189,15,d189,0\1H,17,r190,16,a190,15,d190,0\1H,17,r191,16,a191,15,d191,0\1H,17,r192,16,a192,15,d192,0\1H,17,r193,16,a193,15,d193,0\1H,17,r194,16,a194,15,d194,0\1H,17,r195,16,a195,15,d195,0\1H,17,r196,16,a196,15,d196,0\1H,17,r197,16,a197,15,d197,0\1H,17,r198,16,a198,15,d198,0\1H,17,r199,16,a199,15,d199,0\1H,17,r200,16,a200,15,d200,0\1H,17,r201,16,a201,15,d201,0\1H,17,r202,16,a202,15,d202,0\1H,17,r203,16,a203,15,d203,0\1H,17,r204,16,a204,15,d204,0\1H,17,r205,16,a205,15,d205,0\1H,17,r206,16,a206,15,d206,0\1H,17,r207,16,a207,15,d207,0\1H,17,r208,16,a208,15,d208,0\1H,17,r209,16,a209,15,d209,0\1H,17,r210,16,a210,15,d210,0\1H,17,r211,16,a211,15,d211,0\1H,17,r212,16,a212,15,d212,0\1H,17,r213,16,a213,15,d213,0\1H,17,r214,16,a214,15,d214,0\1H,17,r215,16,a215,15,d215,0\1H,17,r216,16,a216,15,d216,0\1H,17,r217,16,a217,15,d217,0\1H,17,r218,16,a218,15,d218,0\1H,17,r219,16,a219,15,d219,0\1H,17,r220,16,a220,15,d220,0\1H,17,r221,16,a221,15,d221,0\1H,17,r222,16,a222,15,d222,0\1H,17,r223,16,a223,15,d223,0\1H,17,r224,16,a224,15,d224,0\1H,17,r225,16,a225,15,d225,0\1H,17,r226,16,a226,15,d226,0\1H,17,r227,16,a227,15,d227,0\1H,17,r228,16,a228,15,d228,0\1H,17,r229,16,a229,15,d229,0\1H,17,r230,16,a230,15,d230,0\1H,17,r231,16,a231,15,d231,0\1H,17,r232,16,a232,15,d232,0\1H,17,r233,16,a233,15,d233,0\1H,17,r234,16,a234,15,d234,0\1H,17,r235,16,a235,15,d235,0\1H,17,r236,16,a236,15,d236,0\1H,17,r237,16,a237,15,d237,0\1H,17,r238,16,a238,15,d238,0\1H,17,r239,16,a239,15,d239,0\1H,17,r240,16,a240,15,d240,0\1H,17,r241,16,a241,15,d241,0\1H,17,r242,16,a242,15,d242,0\1H,17,r243,16,a243,15,d243,0\1H,17,r244,16,a244,15,d244,0\1H,17,r245,16,a245,15,d245,0\1H,17,r246,16,a246,15,d246,0\1H,17,r247,16,a247,15,d247,0\1H,17,r248,16,a248,15,d248,0\1H,17,r249,16,a249,15,d249,0\1H,17,r250,16,a250,15,d250,0\1H,17,r251,16,a251,15,d251,0\1H,17,r252,16,a252,15,d252,0\1H,17,r253,16,a253,15,d253,0\1H,17,r254,16,a254,15,d254,0\1H,17,r255,16,a255,15,d255,0\1H,17,r256,16,a256,15,d256,0\1H,17,r257,16,a257,15,d257,0\1H,17,r258,16,a258,15,d258,0\1H,17,r259,16,a259,15,d259,0\1H,17,r260,16,a260,15,d260,0\1H,17,r261,16,a261,15,d261,0\1H,17,r262,16,a262,15,d262,0\1H,17,r263,16,a263,15,d263,0\1H,17,r264,16,a264,15,d264,0\1H,17,r265,16,a265,15,d265,0\1H,17,r266,16,a266,15,d266,0\1H,17,r267,16,a267,15,d267,0\1H,17,r268,16,a268,15,d268,0\1H,17,r269,16,a269,15,d269,0\1H,17,r270,16,a270,15,d270,0\1H,17,r271,16,a271,15,d271,0\1H,17,r272,16,a272,15,d272,0\1H,17,r273,16,a273,15,d273,0\1H,17,r274,16,a274,15,d274,0\1H,17,r275,16,a275,15,d275,0\1H,17,r276,16,a276,15,d276,0\1H,17,r277,16,a277,15,d277,0\1H,17,r278,16,a278,15,d278,0\1H,17,r279,16,a279,15,d279,0\1H,17,r280,16,a280,15,d280,0\1H,17,r281,16,a281,15,d281,0\1H,17,r282,16,a282,15,d282,0\1H,17,r283,16,a283,15,d283,0\1H,17,r284,16,a284,15,d284,0\1H,17,r285,16,a285,15,d285,0\1H,17,r286,16,a286,15,d286,0\1H,17,r287,16,a287,15,d287,0\1H,17,r288,16,a288,15,d288,0\1H,17,r289,16,a289,15,d289,0\1H,17,r290,16,a290,15,d290,0\1H,17,r291,16,a291,15,d291,0\1H,17,r292,16,a292,15,d292,0\1H,17,r293,16,a293,15,d293,0\1H,17,r294,16,a294,15,d294,0\1H,17,r295,16,a295,15,d295,0\1H,17,r296,16,a296,15,d296,0\1H,17,r297,16,a297,15,d297,0\1H,17,r298,16,a298,15,d298,0\1H,17,r299,16,a299,15,d299,0\1H,17,r300,16,a300,15,d300,0\1H,17,r301,16,a301,15,d301,0\1H,17,r302,16,a302,15,d302,0\1H,17,r303,16,a303,15,d303,0\1H,17,r304,16,a304,15,d304,0\1H,17,r305,16,a305,15,d305,0\1H,17,r306,16,a306,15,d306,0\1H,17,r307,16,a307,15,d307,0\1H,17,r308,16,a308,15,d308,0\1H,17,r309,16,a309,15,d309,0\1H,17,r310,16,a310,15,d310,0\1H,17,r311,16,a311,15,d311,0\1H,17,r312,16,a312,15,d312,0\1H,17,r313,16,a313,15,d313,0\1H,17,r314,16,a314,15,d314,0\1H,17,r315,16,a315,15,d315,0\1H,17,r316,16,a316,15,d316,0\1H,17,r317,16,a317,15,d317,0\1H,17,r318,16,a318,15,d318,0\1H,17,r319,16,a319,15,d319,0\1H,17,r320,16,a320,15,d320,0\1H,17,r321,16,a321,15,d321,0\1H,17,r322,16,a322,15,d322,0\1H,17,r323,16,a323,15,d323,0\1H,17,r324,16,a324,15,d324,0\1H,17,r325,16,a325,15,d325,0\1H,17,r326,16,a326,15,d326,0\1H,17,r327,16,a327,15,d327,0\1H,17,r328,16,a328,15,d328,0\1H,17,r329,16,a329,15,d329,0\1H,17,r330,16,a330,15,d330,0\1H,17,r331,16,a331,15,d331,0\1H,17,r332,16,a332,15,d332,0\1H,17,r333,16,a333,15,d333,0\1H,17,r334,16,a334,15,d334,0\1H,17,r335,16,a335,15,d335,0\1H,17,r336,16,a336,15,d336,0\1H,17,r337,16,a337,15,d337,0\1H,17,r338,16,a338,15,d338,0\1H,17,r339,16,a339,15,d339,0\1H,17,r340,16,a340,15,d340,0\1H,17,r341,16,a341,15,d341,0\1H,17,r342,16,a342,15,d342,0\1H,17,r343,16,a343,15,d343,0\1H,17,r344,16,a344,15,d344,0\1H,17,r345,16,a345,15,d345,0\1H,17,r346,16,a346,15,d346,0\1H,17,r347,16,a347,15,d347,0\1H,17,r348,16,a348,15,d348,0\1H,17,r349,16,a349,15,d349,0\1H,17,r350,16,a350,15,d350,0\1H,17,r351,16,a351,15,d351,0\1H,17,r352,16,a352,15,d352,0\1H,17,r353,16,a353,15,d353,0\1H,17,r354,16,a354,15,d354,0\1H,17,r355,16,a355,15,d355,0\1H,17,r356,16,a356,15,d356,0\1H,17,r357,16,a357,15,d357,0\1H,17,r358,16,a358,15,d358,0\1H,17,r359,16,a359,15,d359,0\1H,17,r360,16,a360,15,d360,0\1H,17,r361,16,a361,15,d361,0\1H,17,r362,16,a362,15,d362,0\1H,17,r363,16,a363,15,d363,0\1H,17,r364,16,a364,15,d364,0\1H,17,r365,16,a365,15,d365,0\1H,17,r366,16,a366,15,d366,0\1H,17,r367,16,a367,15,d367,0\1H,17,r368,16,a368,15,d368,0\1H,17,r369,16,a369,15,d369,0\1H,17,r370,16,a370,15,d370,0\1H,17,r371,16,a371,15,d371,0\1H,17,r372,16,a372,15,d372,0\1H,17,r373,16,a373,15,d373,0\1H,17,r374,16,a374,15,d374,0\1H,17,r375,16,a375,15,d375,0\1H,17,r376,16,a376,15,d376,0\1H,17,r377,16,a377,15,d377,0\1H,17,r378,16,a378,15,d378,0\1H,17,r379,16,a379,15,d379,0\1H,17,r380,16,a380,15,d380,0\1H,17,r381,16,a381,15,d381,0\1H,17,r382,16,a382,15,d382,0\1H,17,r383,16,a383,15,d383,0\1H,17,r384,16,a384,15,d384,0\1H,17,r385,16,a385,15,d385,0\1H,17,r386,16,a386,15,d386,0\1H,17,r387,16,a387,15,d387,0\1H,17,r388,16,a388,15,d388,0\1H,17,r389,16,a389,15,d389,0\1H,17,r390,16,a390,15,d390,0\1H,17,r391,16,a391,15,d391,0\1H,17,r392,16,a392,15,d392,0\1H,17,r393,16,a393,15,d393,0\1H,17,r394,16,a394,15,d394,0\1H,17,r395,16,a395,15,d395,0\1H,17,r396,16,a396,15,d396,0\1H,17,r397,16,a397,15,d397,0\1H,17,r398,16,a398,15,d398,0\1H,17,r399,16,a399,15,d399,0\1H,17,r400,16,a400,15,d400,0\1H,17,r401,16,a401,15,d401,0\1H,17,r402,16,a402,15,d402,0\1H,17,r403,16,a403,15,d403,0\1H,17,r404,16,a404,15,d404,0\1H,17,r405,16,a405,15,d405,0\1H,17,r406,16,a406,15,d406,0\1H,17,r407,16,a407,15,d407,0\1H,17,r408,16,a408,15,d408,0\1H,17,r409,16,a409,15,d409,0\1H,17,r410,16,a410,15,d410,0\1H,17,r411,16,a411,15,d411,0\1H,17,r412,16,a412,15,d412,0\1H,17,r413,16,a413,15,d413,0\1H,17,r414,16,a414,15,d414,0\1H,17,r415,16,a415,15,d415,0\1H,17,r416,16,a416,15,d416,0\1H,17,r417,16,a417,15,d417,0\1H,17,r418,16,a418,15,d418,0\1H,17,r419,16,a419,15,d419,0\1H,17,r420,16,a420,15,d420,0\1H,17,r421,16,a421,15,d421,0\1H,17,r422,16,a422,15,d422,0\1H,17,r423,16,a423,15,d423,0\1H,17,r424,16,a424,15,d424,0\1H,17,r425,16,a425,15,d425,0\1H,17,r426,16,a426,15,d426,0\1H,17,r427,16,a427,15,d427,0\1H,17,r428,16,a428,15,d428,0\1H,17,r429,16,a429,15,d429,0\1H,17,r430,16,a430,15,d430,0\1H,17,r431,16,a431,15,d431,0\1H,17,r432,16,a432,15,d432,0\1H,17,r433,16,a433,15,d433,0\1H,17,r434,16,a434,15,d434,0\1H,17,r435,16,a435,15,d435,0\1H,17,r436,16,a436,15,d436,0\1H,17,r437,16,a437,15,d437,0\1H,17,r438,16,a438,15,d438,0\1H,17,r439,16,a439,15,d439,0\1H,17,r440,16,a440,15,d440,0\1H,17,r441,16,a441,15,d441,0\1H,17,r442,16,a442,15,d442,0\1H,17,r443,16,a443,15,d443,0\1H,17,r444,16,a444,15,d444,0\1H,17,r445,16,a445,15,d445,0\1H,17,r446,16,a446,15,d446,0\1H,17,r447,16,a447,15,d447,0\1H,17,r448,16,a448,15,d448,0\1H,17,r449,16,a449,15,d449,0\1H,17,r450,16,a450,15,d450,0\1H,17,r451,1

Sparteine 1b (energy minimum 1)

Item Value Threshold Converged?
 Maximum Force .000147 .000450 YES
 RMS Force .000032 .000300 YES
 Maximum Displacement .000327 .001800 YES
 RMS Displacement .000088 .001200 YES
 Predicted change in Energy=-2.535924D-08
 Optimization completed.
 -- Stationary point found.

 ! Optimized Parameters !
 ! (Angstroms and Degrees) !

! Name	Value	Derivative information (Atomic Units)	!
! r2	1.5371	-DE/DX = 0.	!
! r3	1.5266	-DE/DX = 0.	!
! a3	111.0991	-DE/DX = -0.0001	!
! r4	1.5248	-DE/DX = 0.	!
! a4	106.3628	-DE/DX = -0.0001	!
! d4	299.5418	-DE/DX = 0.0001	!
! r5	1.5293	-DE/DX = 0.	!
! a5	107.9328	-DE/DX = -0.0001	!
! d5	64.134	-DE/DX = 0.0001	!
! r6	1.4552	-DE/DX = 0.	!
! a6	110.762	-DE/DX = 0.	!
! d6	298.271	-DE/DX = 0.	!
! r7	1.5272	-DE/DX = 0.	!
! a7	113.3939	-DE/DX = 0.	!
! d7	238.4641	-DE/DX = 0.0001	!
! r8	1.5386	-DE/DX = 0.	!
! a8	109.5113	-DE/DX = -0.0001	!
! d8	297.8571	-DE/DX = 0.	!
! r9	1.458	-DE/DX = 0.	!
! a9	112.7438	-DE/DX = 0.	!
! d9	63.4398	-DE/DX = 0.0001	!
! r10	1.5393	-DE/DX = 0.	!
! a10	111.8487	-DE/DX = 0.0001	!
! d10	285.4022	-DE/DX = 0.0001	!
! r11	1.5296	-DE/DX = 0.	!
! a11	110.9378	-DE/DX = -0.0001	!
! d11	180.6026	-DE/DX = 0.	!
! r12	1.528	-DE/DX = 0.	!
! a12	110.4326	-DE/DX = 0.	!
! d12	305.8075	-DE/DX = 0.	!
! r13	1.4599	-DE/DX = 0.	!
! a13	113.7971	-DE/DX = 0.	!
! d13	184.4365	-DE/DX = -0.0001	!
! r14	1.4603	-DE/DX = 0.	!
! a14	109.7458	-DE/DX = 0.0001	!
! d14	175.764	-DE/DX = 0.	!
! r15	1.5269	-DE/DX = 0.	!
! a15	112.4675	-DE/DX = 0.0001	!
! d15	177.9083	-DE/DX = 0.	!
! r16	1.5227	-DE/DX = 0.	!
! a16	110.9869	-DE/DX = -0.0001	!
! d16	172.1246	-DE/DX = 0.0001	!
! r17	1.5256	-DE/DX = 0.	!
! a17	110.2554	-DE/DX = 0.	!
! d17	56.9396	-DE/DX = 0.	!
! r18	1.1037	-DE/DX = 0.	!
! a18	107.6341	-DE/DX = 0.	!
! d18	168.0124	-DE/DX = 0.	!
! r19	1.1001	-DE/DX = 0.	!
! a19	107.2468	-DE/DX = 0.	!
! d19	120.3657	-DE/DX = 0.	!
! r20	1.0969	-DE/DX = 0.	!
! a20	112.0384	-DE/DX = 0.	!
! d20	60.5869	-DE/DX = 0.	!

!	r21	1.0985	-DE/DX = 0.	!
!	a21	109.9033	-DE/DX = 0.	!
!	d21	179.5251	-DE/DX = 0.	!
!	r22	1.1004	-DE/DX = 0.	!
!	a22	110.0003	-DE/DX = 0.	!
!	d22	181.196	-DE/DX = 0.	!
!	r23	1.1094	-DE/DX = 0.	!
!	a23	107.2507	-DE/DX = 0.	!
!	d23	63.5389	-DE/DX = 0.	!
!	r24	1.0967	-DE/DX = 0.	!
!	a24	110.8961	-DE/DX = 0.	!
!	d24	179.0662	-DE/DX = 0.	!
!	r25	1.1125	-DE/DX = 0.	!
!	a25	107.8651	-DE/DX = 0.	!
!	d25	186.9785	-DE/DX = 0.	!
!	r26	1.0985	-DE/DX = 0.	!
!	a26	110.1583	-DE/DX = 0.	!
!	d26	303.1917	-DE/DX = 0.	!
!	r27	1.0982	-DE/DX = 0.	!
!	a27	109.4024	-DE/DX = 0.	!
!	d27	302.7069	-DE/DX = 0.	!
!	r28	1.0972	-DE/DX = 0.	!
!	a28	110.0153	-DE/DX = 0.	!
!	d28	59.6963	-DE/DX = 0.	!
!	r29	1.0993	-DE/DX = 0.	!
!	a29	109.1168	-DE/DX = 0.	!
!	d29	65.6392	-DE/DX = 0.	!
!	r30	1.0967	-DE/DX = 0.	!
!	a30	110.5371	-DE/DX = 0.	!
!	d30	182.6691	-DE/DX = 0.	!
!	r31	1.0976	-DE/DX = 0.	!
!	a31	110.8306	-DE/DX = 0.	!
!	d31	175.5568	-DE/DX = 0.	!
!	r32	1.0975	-DE/DX = 0.	!
!	a32	109.7352	-DE/DX = 0.	!
!	d32	293.3121	-DE/DX = 0.	!
!	r33	1.1001	-DE/DX = 0.	!
!	a33	107.3577	-DE/DX = 0.	!
!	d33	163.0817	-DE/DX = 0.	!
!	r34	1.0972	-DE/DX = 0.	!
!	a34	107.9353	-DE/DX = 0.	!
!	d34	48.0028	-DE/DX = 0.	!
!	r35	1.1165	-DE/DX = 0.	!
!	a35	105.5967	-DE/DX = 0.	!
!	d35	294.9951	-DE/DX = 0.	!
!	r36	1.1115	-DE/DX = 0.	!
!	a36	111.1905	-DE/DX = 0.	!
!	d36	294.4023	-DE/DX = 0.	!
!	r37	1.0969	-DE/DX = 0.	!
!	a37	107.8487	-DE/DX = 0.	!
!	d37	51.3789	-DE/DX = 0.	!
!	r38	1.0956	-DE/DX = 0.	!
!	a38	108.0942	-DE/DX = 0.	!
!	d38	294.8705	-DE/DX = 0.	!
!	r39	1.0983	-DE/DX = 0.	!
!	a39	109.4555	-DE/DX = 0.	!
!	d39	52.3006	-DE/DX = 0.	!
!	r40	1.0971	-DE/DX = 0.	!
!	a40	109.747	-DE/DX = 0.	!
!	d40	179.495	-DE/DX = 0.	!
!	r41	1.0961	-DE/DX = 0.	!
!	a41	108.4724	-DE/DX = 0.	!
!	d41	296.8049	-DE/DX = 0.	!
!	r42	1.0967	-DE/DX = 0.	!
!	a42	110.8288	-DE/DX = 0.	!
!	d42	184.4731	-DE/DX = 0.	!
!	r43	1.0986	-DE/DX = 0.	!
!	a43	109.3909	-DE/DX = 0.	!
!	d43	66.9015	-DE/DX = 0.	!

```

1\1\GINC-ARMON\FOpt\RMP2-FC\6-31G(d)\C15H26N2\BELOSTOT\17-Feb-2002\1\
# MP2/6-31G* GEOM=ALLCHECKPOINT GUESS=CHECKPOINT OPT=Z-MATRIX\Spartei
ne, the minimal energy conformer\0,1\C\1,1,r2\C,2,r3,1,a3\C,3,r4,2,a4
,1,d4,0\C,4,r5,3,a5,2,d5,0\N,5,r6,4,a6,3,d6,0\C,2,r7,1,a7,3,d7,0\C,4,r
8,3,a8,2,d8,0\N,7,r9,2,a9,1,d9,0\C,1,r10,2,a10,3,d10,0\C,10,r11,1,a11,
2,d11,0\C,11,r12,10,a12,1,d12,0\C,6,r13,5,a13,4,d13,0\C,9,r14,7,a14,2,
d14,0\C,8,r15,4,a15,3,d15,0\C,14,r16,9,a16,7,d16,0\C,16,r17,14,a17,9,d
17,0\H,1,r18,2,a18,3,d18,0\H,2,r19,1,a19,3,d19,0\H,3,r20,2,a20,1,d20,0
\H,3,r21,2,a21,1,d21,0\H,4,r22,3,a22,2,d22,0\H,5,r23,4,a23,3,d23,0\H,5
,r24,4,a24,3,d24,0\H,7,r25,2,a25,1,d25,0\H,7,r26,2,a26,1,d26,0\H,10,r2
7,1,a27,2,d27,0\H,10,r28,1,a28,2,d28,0\H,11,r29,10,a29,1,d29,0\H,11,r3
0,10,a30,1,d30,0\H,12,r31,11,a31,10,d31,0\H,12,r32,11,a32,10,d32,0\H,1
3,r33,6,a33,5,d33,0\H,13,r34,6,a34,5,d34,0\H,8,r35,4,a35,3,d35,0\H,14,
r36,9,a36,7,d36,0\H,14,r37,9,a37,7,d37,0\H,15,r38,8,a38,4,d38,0\H,15,r
39,8,a39,4,d39,0\H,16,r40,14,a40,9,d40,0\H,16,r41,14,a41,9,d41,0\H,17,
r42,16,a42,14,d42,0\H,17,r43,16,a43,14,d43,0\H,17,r44,16,a44,14,d44,0\
H,17,r45,16,a45,14,d45,0\H,17,r46,16,a46,14,d46,0\H,17,r47,16,a47,14,d47,0\
H,17,r48,16,a48,14,d48,0\H,17,r49,16,a49,14,d49,0\H,17,r50,16,a50,14,d50,0\
H,17,r51,16,a51,14,d51,0\H,17,r52,16,a52,14,d52,0\H,17,r53,16,a53,14,d53,0\
H,17,r54,16,a54,14,d54,0\H,17,r55,16,a55,14,d55,0\H,17,r56,16,a56,14,d56,0\
H,17,r57,16,a57,14,d57,0\H,17,r58,16,a58,14,d58,0\H,17,r59,16,a59,14,d59,0\
H,17,r60,16,a60,14,d60,0\H,17,r61,16,a61,14,d61,0\H,17,r62,16,a62,14,d62,0\
H,17,r63,16,a63,14,d63,0\H,17,r64,16,a64,14,d64,0\H,17,r65,16,a65,14,d65,0\
H,17,r66,16,a66,14,d66,0\H,17,r67,16,a67,14,d67,0\H,17,r68,16,a68,14,d68,0\
H,17,r69,16,a69,14,d69,0\H,17,r70,16,a70,14,d70,0\H,17,r71,16,a71,14,d71,0\
H,17,r72,16,a72,14,d72,0\H,17,r73,16,a73,14,d73,0\H,17,r74,16,a74,14,d74,0\
H,17,r75,16,a75,14,d75,0\H,17,r76,16,a76,14,d76,0\H,17,r77,16,a77,14,d77,0\
H,17,r78,16,a78,14,d78,0\H,17,r79,16,a79,14,d79,0\H,17,r80,16,a80,14,d80,0\
H,17,r81,16,a81,14,d81,0\H,17,r82,16,a82,14,d82,0\H,17,r83,16,a83,14,d83,0\
H,17,r84,16,a84,14,d84,0\H,17,r85,16,a85,14,d85,0\H,17,r86,16,a86,14,d86,0\
H,17,r87,16,a87,14,d87,0\H,17,r88,16,a88,14,d88,0\H,17,r89,16,a89,14,d89,0\
H,17,r90,16,a90,14,d90,0\H,17,r91,16,a91,14,d91,0\H,17,r92,16,a92,14,d92,0\
H,17,r93,16,a93,14,d93,0\H,17,r94,16,a94,14,d94,0\H,17,r95,16,a95,14,d95,0\
H,17,r96,16,a96,14,d96,0\H,17,r97,16,a97,14,d97,0\H,17,r98,16,a98,14,d98,0\
H,17,r99,16,a99,14,d99,0\H,17,r100,16,a100,14,d100,0\H,17,r101,16,a101,14,d101,0\
H,17,r102,16,a102,14,d102,0\H,17,r103,16,a103,14,d103,0\H,17,r104,16,a104,14,d104,0\
H,17,r105,16,a105,14,d105,0\H,17,r106,16,a106,14,d106,0\H,17,r107,16,a107,14,d107,0\
H,17,r108,16,a108,14,d108,0\H,17,r109,16,a109,14,d109,0\H,17,r110,16,a110,14,d110,0\
H,17,r111,16,a111,14,d111,0\H,17,r112,16,a112,14,d112,0\H,17,r113,16,a113,14,d113,0\
H,17,r114,16,a114,14,d114,0\H,17,r115,16,a115,14,d115,0\H,17,r116,16,a116,14,d116,0\
H,17,r117,16,a117,14,d117,0\H,17,r118,16,a118,14,d118,0\H,17,r119,16,a119,14,d119,0\
H,17,r120,16,a120,14,d120,0\H,17,r121,16,a121,14,d121,0\H,17,r122,16,a122,14,d122,0\
H,17,r123,16,a123,14,d123,0\H,17,r124,16,a124,14,d124,0\H,17,r125,16,a125,14,d125,0\
H,17,r126,16,a126,14,d126,0\H,17,r127,16,a127,14,d127,0\H,17,r128,16,a128,14,d128,0\
H,17,r129,16,a129,14,d129,0\H,17,r130,16,a130,14,d130,0\H,17,r131,16,a131,14,d131,0\
H,17,r132,16,a132,14,d132,0\H,17,r133,16,a133,14,d133,0\H,17,r134,16,a134,14,d134,0\
H,17,r135,16,a135,14,d135,0\H,17,r136,16,a136,14,d136,0\H,17,r137,16,a137,14,d137,0\
H,17,r138,16,a138,14,d138,0\H,17,r139,16,a139,14,d139,0\H,17,r140,16,a140,14,d140,0\
H,17,r141,16,a141,14,d141,0\H,17,r142,16,a142,14,d142,0\H,17,r143,16,a143,14,d143,0\
H,17,r144,16,a144,14,d144,0\H,17,r145,16,a145,14,d145,0\H,17,r146,16,a146,14,d146,0\
H,17,r147,16,a147,14,d147,0\H,17,r148,16,a148,14,d148,0\H,17,r149,16,a149,14,d149,0\
H,17,r150,16,a150,14,d150,0\H,17,r151,16,a151,14,d151,0\H,17,r152,16,a152,14,d152,0\
H,17,r153,16,a153,14,d153,0\H,17,r154,16,a154,14,d154,0\H,17,r155,16,a155,14,d155,0\
H,17,r156,16,a156,14,d156,0\H,17,r157,16,a157,14,d157,0\H,17,r158,16,a158,14,d158,0\
H,17,r159,16,a159,14,d159,0\H,17,r160,16,a160,14,d160,0\H,17,r161,16,a161,14,d161,0\
H,17,r162,16,a162,14,d162,0\H,17,r163,16,a163,14,d163,0\H,17,r164,16,a164,14,d164,0\
H,17,r165,16,a165,14,d165,0\H,17,r166,16,a166,14,d166,0\H,17,r167,16,a167,14,d167,0\
H,17,r168,16,a168,14,d168,0\H,17,r169,16,a169,14,d169,0\H,17,r170,16,a170,14,d170,0\
H,17,r171,16,a171,14,d171,0\H,17,r172,16,a172,14,d172,0\H,17,r173,16,a173,14,d173,0\
H,17,r174,16,a174,14,d174,0\H,17,r175,16,a175,14,d175,0\H,17,r176,16,a176,14,d176,0\
H,17,r177,16,a177,14,d177,0\H,17,r178,16,a178,14,d178,0\H,17,r179,16,a179,14,d179,0\
H,17,r180,16,a180,14,d180,0\H,17,r181,16,a181,14,d181,0\H,17,r182,16,a182,14,d182,0\
H,17,r183,16,a183,14,d183,0\H,17,r184,16,a184,14,d184,0\H,17,r185,16,a185,14,d185,0\
H,17,r186,16,a186,14,d186,0\H,17,r187,16,a187,14,d187,0\H,17,r188,16,a188,14,d188,0\
H,17,r189,16,a189,14,d189,0\H,17,r190,16,a190,14,d190,0\H,17,r191,16,a191,14,d191,0\
H,17,r192,16,a192,14,d192,0\H,17,r193,16,a193,14,d193,0\H,17,r194,16,a194,14,d194,0\
H,17,r195,16,a195,14,d195,0\H,17,r196,16,a196,14,d196,0\H,17,r197,16,a197,14,d197,0\
H,17,r198,16,a198,14,d198,0\H,17,r199,16,a199,14,d199,0\H,17,r200,16,a200,14,d200,0\
H,17,r201,16,a201,14,d201,0\H,17,r202,16,a202,14,d202,0\H,17,r203,16,a203,14,d203,0\
H,17,r204,16,a204,14,d204,0\H,17,r205,16,a205,14,d205,0\H,17,r206,16,a206,14,d206,0\
H,17,r207,16,a207,14,d207,0\H,17,r208,16,a208,14,d208,0\H,17,r209,16,a209,14,d209,0\
H,17,r210,16,a210,14,d210,0\H,17,r211,16,a211,14,d211,0\H,17,r212,16,a212,14,d212,0\
H,17,r213,16,a213,14,d213,0\H,17,r214,16,a214,14,d214,0\H,17,r215,16,a215,14,d215,0\
H,17,r216,16,a216,14,d216,0\H,17,r217,16,a217,14,d217,0\H,17,r218,16,a218,14,d218,0\
H,17,r219,16,a219,14,d219,0\H,17,r220,16,a220,14,d220,0\H,17,r221,16,a221,14,d221,0\
H,17,r222,16,a222,14,d222,0\H,17,r223,16,a223,14,d223,0\H,17,r224,16,a224,14,d224,0\
H,17,r225,16,a225,14,d225,0\H,17,r226,16,a226,14,d226,0\H,17,r227,16,a227,14,d227,0\
H,17,r228,16,a228,14,d228,0\H,17,r229,16,a229,14,d229,0\H,17,r230,16,a230,14,d230,0\
H,17,r231,16,a231,14,d231,0\H,17,r232,16,a232,14,d232,0\H,17,r233,16,a233,14,d233,0\
H,17,r234,16,a234,14,d234,0\H,17,r235,16,a235,14,d235,0\H,17,r236,16,a236,14,d236,0\
H,17,r237,16,a237,14,d237,0\H,17,r238,16,a238,14,d238,0\H,17,r239,16,a239,14,d239,0\
H,17,r240,16,a240,14,d240,0\H,17,r241,16,a241,14,d241,0\H,17,r242,16,a242,14,d242,0\
H,17,r243,16,a243,14,d243,0\H,17,r244,16,a244,14,d244,0\H,17,r245,16,a245,14,d245,0\
H,17,r246,16,a246,14,d246,0\H,17,r247,16,a247,14,d247,0\H,17,r248,16,a248,14,d248,0\
H,17,r249,16,a249,14,d249,0\H,17,r250,16,a250,14,d250,0\H,17,r251,16,a251,14,d251,0\
H,17,r252,16,a252,14,d252,0\H,17,r253,16,a253,14,d253,0\H,17,r254,16,a254,14,d254,0\
H,17,r255,16,a255,14,d255,0\H,17,r256,16,a256,14,d256,0\H,17,r257,16,a257,14,d257,0\
H,17,r258,16,a258,14,d258,0\H,17,r259,16,a259,14,d259,0\H,17,r260,16,a260,14,d260,0\
H,17,r261,16,a261,14,d261,0\H,17,r262,16,a262,14,d262,0\H,17,r263,16,a263,14,d263,0\
H,17,r264,16,a264,14,d264,0\H,17,r265,16,a265,14,d265,0\H,17,r266,16,a266,14,d266,0\
H,17,r267,16,a267,14,d267,0\H,17,r268,16,a268,14,d268,0\H,17,r269,16,a269,14,d269,0\
H,17,r270,16,a270,14,d270,0\H,17,r271,16,a271,14,d271,0\H,17,r272,16,a272,14,d272,0\
H,17,r273,16,a273,14,d273,0\H,17,r274,16,a274,14,d274,0\H,17,r275,16,a275,14,d275,0\
H,17,r276,16,a276,14,d276,0\H,17,r277,16,a277,14,d277,0\H,17,r278,16,a278,14,d278,0\
H,17,r279,16,a279,14,d279,0\H,17,r280,16,a280,14,d280,0\H,17,r281,16,a281,14,d281,0\
H,17,r282,16,a282,14,d282,0\H,17,r283,16,a283,14,d283,0\H,17,r284,16,a284,14,d284,0\
H,17,r285,16,a285,14,d285,0\H,17,r286,16,a286,14,d286,0\H,17,r287,16,a287,14,d287,0\
H,17,r288,16,a288,14,d288,0\H,17,r289,16,a289,14,d289,0\H,17,r290,16,a290,14,d290,0\
H,17,r291,16,a291,14,d291,0\H,17,r292,16,a292,14,d292,0\H,17,r293,16,a293,14,d293,0\
H,17,r294,16,a294,14,d294,0\H,17,r295,16,a295,14,d295,0\H,17,r296,16,a296,14,d296,0\
H,17,r297,16,a297,14,d297,0\H,17,r298,16,a298,14,d298,0\H,17,r299,16,a299,14,d299,0\
H,17,r300,16,a300,14,d300,0\H,17,r301,16,a301,14,d301,0\H,17,r302,16,a302,14,d302,0\
H,17,r303,16,a303,14,d303,0\H,17,r304,16,a304,14,d304,0\H,17,r305,16,a305,14,d305,0\
H,17,r306,16,a306,14,d306,0\H,17,r307,16,a307,14,d307,0\H,17,r308,16,a308,14,d308,0\
H,17,r309,16,a309,14,d309,0\H,17,r310,16,a310,14,d310,0\H,17,r311,16,a311,14,d311,0\
H,17,r312,16,a312,14,d312,0\H,17,r313,16,a313,14,d313,0\H,17,r314,16,a314,14,d314,0\
H,17,r315,16,a315,14,d315,0\H,17,r316,16,a316,14,d316,0\H,17,r317,16,a317,14,d317,0\
H,17,r318,16,a318,14,d318,0\H,17,r319,16,a319,14,d319,0\H,17,r320,16,a320,14,d320,0\
H,17,r321,16,a321,14,d321,0\H,17,r322,16,a322,14,d322,0\H,17,r323,16,a323,14,d323,0\
H,17,r324,16,a324,14,d324,0\H,17,r325,16,a325,14,d325,0\H,17,r326,16,a326,14,d326,0\
H,17,r327,16,a327,14,d327,0\H,17,r328,16,a328,14,d328,0\H,17,r329,16,a329,14,d329,0\
H,17,r330,16,a330,14,d330,0\H,17,r331,16,a331,14,d331,0\H,17,r332,16,a332,14,d332,0\
H,17,r333,16,a333,14,d333,0\H,17,r334,16,a334,14,d334,0\H,17,r335,16,a335,14,d335,0\
H,17,r336,16,a336,14,d336,0\H,17,r337,16,a337,14,d337,0\H,17,r338,16,a338,14,d338,0\
H,17,r339,16,a339,14,d339,0\H,17,r340,16,a340,14,d340,0\H,17,r341,16,a341,14,d341,0\
H,17,r342,16,a342,14,d342,0\H,17,r343,16,a343,14,d343,0\H,17,r344,16,a344,14,d344,0\
H,17,r345,16,a345,14,d345,0\H,17,r346,16,a346,14,d346,0\H,17,r347,16,a347,14,d347,0\
H,17,r348,16,a348,14,d348,0\H,17,r349,16,a349,14,d349,0\H,17,r350,16,a350,14,d350,0\
H,17,r351,16,a351,14,d351,0\H,17,r352,16,a352,14,d352,0\H,17,r353,16,a353,14,d353,0\
H,17,r354,16,a354,14,d354,0\H,17,r355,16,a355,14,d355,0\H,17,r356,16,a356,14,d356,0\
H,17,r357,16,a357,14,d357,0\H,17,r358,16,a358,14,d358,0\H,17,r359,16,a359,14,d359,0\
H,17,r360,16,a360,14,d360,0\H,17,r361,16,a361,14,d361,0\H,17,r362,16,a362,14,d362,0\
H,17,r363,16,a363,14,d363,0\H,17,r364,16,a364,14,d364,0\H,17,r365,16,a365,14,d365,0\
H,17,r366,16,a366,14,d366,0\H,17,r367,16,a367,14,d367,0\H,17,r368,16,a368,14,d368,0\
H,17,r369,16,a369,14,d369,0\H,17,r370,16,a370,14,d370,0\H,17,r371,16,a371,14,d371,0\
H,17,r372,16,a372,14,d372,0\H,17,r373,16,a373,14,d373,0\H,17,r374,16,a374,14,d374,0\
H,17,r375,16,a375,14,d375,0\H,17,r376,16,a376,14,d376,0\H,17,r377,16,a377,14,d377,0\
H,17,r378,16,a378,14,d378,0\H,17,r379,16,a379,14,d379,0\H,17,r380,16,a380,14,d380,0\
H,17,r381,16,a381,14,d381,0\H,17,r382,16,a382,14,d382,0\H,17,r383,16,a383,14,d383,0\
H,17,r384,16,a384,14,d384,0\H,17,r385,16,a385,14,d385,0\H,17,r386,16,a386,14,d386,0\
H,17,r387,16,a387,14,d387,0\H,17,r388,16,a388,14,d388,0\H,17,r389,16,a389,14,d389,0\
H,17,r390,16,a390,14,d390,0\H,17,r391,16,a391,14,d391,0\H,17,r392,16,a392,14,d392,0\
H,17,r393,16,a393,14,d393,0\H,17,r394,16,a394,14,d394,0\H,17,r395,16,a395,14,d395,0\
H,17,r396,16,a396,14,d396,0\H,17,r397,16,a397,14,d397,0\H,17,r398,16,a398,14,d398,0\
H,17,r399,16,a399,14,d399,0\H,17,r400,16,a400,14,d400,0\H,17,r401,16,a401,14,d401,0\
H,17,r402,16,a402,14,d402,0\H,17,r403,16,a403,14,d403,0\H,17,r404,16,a404,14,d404,0\
H,17,r405,16,a405,14,d405,0\H,17,r406,16,a406,14,d406,0\H,17,r407,16,a407,14,d407,0\
H,17,r408,16,a408,14,d408,0\H,17,r409,16,a409,14,d409,0\H,17,r410,16,a410,14,d410,0\
H,17,r411,16,a411,14,d411,0\H,17,r412,16,a412,14,d412,0\H,17,r413,16,a413,14,d413,0\
H,17,r414,16,a414,14,d414,0\H,17,r415,16,a415,14,d415,0\H,17,r416,16,a416,14,d416,0\
H,17,r417,16,a417,14,d417,0\H,17,r418,16,a418,14,d418,0\H,17,r419,16,a419,14,d419,0\
H,17,r420,16,a420,14,d420,0\H,17,r421,16,a421,14,d421,0\H,17,r422,16,a422,14,d422,0\
H,17,r423,16,a423,14,d423,0\H,17,r424,16,a424,14,d424,0\H,17,r425,16,a425,14,d425,0\
H,17,r426,16,a426,14,d426,0\H,17,r427,16,a427,14,d427,0\H,17,r428,16,a428,14,d428,0\
H,17,r429,16,a429,14,d429,0\H,17,r430,16,a430,14,d430,0\H,17,r431,16,a431,14,d431,0\
H,17,r432,16,a432,14,d432,0\H,17,r433,16,a433,14,d433,0\H,17,r434,16,a434,14,d434,0\
H,17,r435,16,a435,14,d435,0\H,17,r436,16,a436,14,d436,0\H,17,r437,16,a437,14,d437,0\
H,17,r438,16,a438,14,d438,0\H,17,r439,16,a439,14,d439,0\H,17,r440,16,a440,14,d440,0\
H,17,r441,16,a441,14,d441,0\H,17,r442,16,a442,14,d442,0\H,17,r443,16,a443,14,d443,0\
H,17,r444,16,a444,14,d444,0\H,17,r445,16,a445,14,d445,0\H,17,r446,16,a446,14,d446,0\
H,17,r447,16,a447,14,d447,0\H,17,r448,16,a448,14,d448,0\H,17,r449,16,a449,14,d449,0\
H,17,r450,16,a450,14,d450,0\H,17,r451,16,a451,14,d451,0\H,17,r452,16,a452,14,d452,0\
H,17,r453,16,a453,14,d453,0\H,17,r454,16,a454,14,d454,0\H,17,r455,16,a455,14,d455,0\
H,17,r456,16,a456,14,d456,0\H,17,r457,16,a457,14,d457,0\H,17,r458,16,a458,14,d458,0\
H,17,r459,16,a459,14,d459,0\H,17,r460,16,a460,14,d460,0\H,17,r461,16,a461,14,d461,0\
H,17,r462,16,a462,14,d462,0\H,17,r463,16,a463,14,d463,0\H,17,r464,16,a464,14,d464,0\
H,17,r465,16,a465,14,d465,0\H,17,r466,16,a466,14,d466,0\H,17,r467,16,a467,14,d467,0\
H,17,r468,16,a468,14,d468,0\H,17,r469,16,a469,14,d469,0\H,17,r470,16,a470,14,d470,0\
H,17,r471,16,a471,14,d471,0\H,17,r472,16,a472,14,d472,0\H,17,r473,16,a473,14,d473,0\
H,17,r474,16,a474,14,d474,0\H,17,r475,16,a475,14,d475,0\H,17,r476,16,a476,14,d476,0\
H,17,r477,16,a477,14,d477,0\H,17,r478,16,a478,14,d478,0\H,17,r479,16,a479,14,d479,0\
H,17,r480,16,a480,14,d480,0\H,17,r481,16,a481,14,d481,0\H,17,r482,16,a482,14,d482,0\
H,17,r483,16,a483,14,d483,0\H,17,r484,16,a484,14,d484,0\H,17,r485,16,a485,14,d485,0\
H,17,r486,16,a486,14,d486,0\H,17,r487,16,a487,14,d487,0\H,17,r488,16,a488,14,d488,0\
H,17,r489,16,a489,14,d489,0\H,17,r490,16,a490,14,d490,0\H,17,r491,16,a491,14,d491,0\
H,17,r492,16,a492,14,d492,0\H,17,r493,16,a493,14,d493,0\H,17,r494,16,a494,14,d494,0\
H,17,r495,16,a495,14,d495,0\H,17,r496,16,a496,14,d496,0\H,17,r497,16,a497,14,d497,0\
H,17,r498,16,a498,14,d498,0\H,17,r499,16,a499,14,d499,0\H,17,r500,16,a500,14,d500,0\
H,17,r501,16,a501,14,d501,
```


Dipole moment (Debye):

X= -.7900 Y= .3045 Z= -.2001 Tot= .8700

Quadrupole moment (Debye-Ang):

XX= -106.5659 YY= -105.4462 ZZ= -108.1990

XY= .3795 XZ= -1.4138 YZ= .0965

Octapole moment (Debye-Ang**2):

XXX= -4.0210 YYY= -2.5709 ZZZ= -.7637 XYY= .4965

XXY= .7546 XXZ= -4.6654 XZZ= -2.6933 YZZ= .2496

YYZ= -1.2048 XYZ= 3.4981

Hexadecapole moment (Debye-Ang**3):

XXXX= -4206.3841 YYYY= -994.6747 ZZZZ= -781.8351 XXXY= -10.8200

XXYZ= 10.6624 YYYX= -6.4510 YYYZ= -7.8550 ZZZX= 2.6940

ZZZY= -3.9459 XYYX= -866.7011 XXZZ= -829.5968 YYZZ= -292.4920

XXYZ= 4.3452 YYXZ= 1.8130 ZZXZ= -2.2546

N-N= 1.378230528632D+03 E-N= -4.369000993884D+03 KE= 6.912984343965D+02

11\GINC-ARMON\FOpt\RMP2-FC\6-31G(d)\C15H26N2\BELOSTOT\20-Feb-2002\1\

MP2/6-31G* GEOM=ALLCHECKPOINT GUESS=CHECKPOINT OPT=Z-MATRIX\Spartei

ne, the second in energy conformer\0,1\C\1,r2\C,2,r3,1,a3\C,3,r4,2,

a4,1,d4,0\C,4,r5,3,a5,2,d5,0\N,5,r6,4,a6,3,d6,0\C,2,r7,1,a7,3,d7,0\C,4

,r8,3,a8,2,d8,0\N,7,r9,2,a9,1,d9,0\C,1,r10,2,a10,3,d10,0\C,10,r11,1,a1

1,2,d11,0\C,11,r12,10,a12,1,d12,0\C,6,r13,5,a13,4,d13,0\C,9,r14,7,a14,

2,d14,0\C,8,r15,4,a15,3,d15,0\C,14,r16,9,a16,7,d16,0\C,16,r17,14,a17,9

,d17,0\H,1,r18,2,a18,3,d18,0\H,2,r19,1,a19,3,d19,0\H,3,r20,2,a20,1,d20

,0\H,3,r21,2,a21,1,d21,0\H,4,r22,3,a22,2,d22,0\H,5,r23,4,a23,3,d23,0\H

,5,r24,4,a24,3,d24,0\H,7,r25,2,a25,1,d25,0\H,7,r26,2,a26,1,d26,0\H,10,

r27,1,a27,2,d27,0\H,10,r28,1,a28,2,d28,0\H,11,r29,10,a29,1,d29,0\H,11,

r30,10,a30,1,d30,0\H,12,r31,11,a31,10,d31,0\H,12,r32,11,a32,10,d32,0\H

,13,r33,6,a33,5,d33,0\H,13,r34,6,a34,5,d34,0\H,8,r35,4,a35,3,d35,0\H,1

4,r36,9,a36,7,d36,0\H,14,r37,9,a37,7,d37,0\H,15,r38,8,a38,4,d38,0\H,15

,r39,8,a39,4,d39,0\H,16,r40,14,a40,9,d40,0\H,16,r41,14,a41,9,d41,0\H,1

7,r42,16,a42,14,d42,0\H,17,r43,16,a43,14,d43,0\H,17,r44,16,a44,14,d44,0\H,17,r45,16,a45,14,d45,0\H,17,r46,16,a46,14,d46,0\H,17,r47,16,a47,14,d47,0\H,17,r48,16,a48,14,d48,0\H,17,r49,16,a49,14,d49,0\H,17,r50,16,a50,14,d50,0\H,17,r51,16,a51,14,d51,0\H,17,r52,16,a52,14,d52,0\H,17,r53,16,a53,14,d53,0\H,17,r54,16,a54,14,d54,0\H,17,r55,16,a55,14,d55,0\H,17,r56,16,a56,14,d56,0\H,17,r57,16,a57,14,d57,0\H,17,r58,16,a58,14,d58,0\H,17,r59,16,a59,14,d59,0\H,17,r60,16,a60,14,d60,0\H,17,r61,16,a61,14,d61,0\H,17,r62,16,a62,14,d62,0\H,17,r63,16,a63,14,d63,0\H,17,r64,16,a64,14,d64,0\H,17,r65,16,a65,14,d65,0\H,17,r66,16,a66,14,d66,0\H,17,r67,16,a67,14,d67,0\H,17,r68,16,a68,14,d68,0\H,17,r69,16,a69,14,d69,0\H,17,r70,16,a70,14,d70,0\H,17,r71,16,a71,14,d71,0\H,17,r72,16,a72,14,d72,0\H,17,r73,16,a73,14,d73,0\H,17,r74,16,a74,14,d74,0\H,17,r75,16,a75,14,d75,0\H,17,r76,16,a76,14,d76,0\H,17,r77,16,a77,14,d77,0\H,17,r78,16,a78,14,d78,0\H,17,r79,16,a79,14,d79,0\H,17,r80,16,a80,14,d80,0\H,17,r81,16,a81,14,d81,0\H,17,r82,16,a82,14,d82,0\H,17,r83,16,a83,14,d83,0\H,17,r84,16,a84,14,d84,0\H,17,r85,16,a85,14,d85,0\H,17,r86,16,a86,14,d86,0\H,17,r87,16,a87,14,d87,0\H,17,r88,16,a88,14,d88,0\H,17,r89,16,a89,14,d89,0\H,17,r90,16,a90,14,d90,0\H,17,r91,16,a91,14,d91,0\H,17,r92,16,a92,14,d92,0\H,17,r93,16,a93,14,d93,0\H,17,r94,16,a94,14,d94,0\H,17,r95,16,a95,14,d95,0\H,17,r96,16,a96,14,d96,0\H,17,r97,16,a97,14,d97,0\H,17,r98,16,a98,14,d98,0\H,17,r99,16,a99,14,d99,0\H,17,r100,16,a100,14,d100,0\H,17,r101,16,a101,14,d101,0\H,17,r102,16,a102,14,d102,0\H,17,r103,16,a103,14,d103,0\H,17,r104,16,a104,14,d104,0\H,17,r105,16,a105,14,d105,0\H,17,r106,16,a106,14,d106,0\H,17,r107,16,a107,14,d107,0\H,17,r108,16,a108,14,d108,0\H,17,r109,16,a109,14,d109,0\H,17,r110,16,a110,14,d110,0\H,17,r111,16,a111,14,d111,0\H,17,r112,16,a112,14,d112,0\H,17,r113,16,a113,14,d113,0\H,17,r114,16,a114,14,d114,0\H,17,r115,16,a115,14,d115,0\H,17,r116,16,a116,14,d116,0\H,17,r117,16,a117,14,d117,0\H,17,r118,16,a118,14,d118,0\H,17,r119,16,a119,14,d119,0\H,17,r120,16,a120,14,d120,0\H,17,r121,16,a121,14,d121,0\H,17,r122,16,a122,14,d122,0\H,17,r123,16,a123,14,d123,0\H,17,r124,16,a124,14,d124,0\H,17,r125,16,a125,14,d125,0\H,17,r126,16,a126,14,d126,0\H,17,r127,16,a127,14,d127,0\H,17,r128,16,a128,14,d128,0\H,17,r129,16,a129,14,d129,0\H,17,r130,16,a130,14,d130,0\H,17,r131,16,a131,14,d131,0\H,17,r132,16,a132,14,d132,0\H,17,r133,16,a133,14,d133,0\H,17,r134,16,a134,14,d134,0\H,17,r135,16,a135,14,d135,0\H,17,r136,16,a136,14,d136,0\H,17,r137,16,a137,14,d137,0\H,17,r138,16,a138,14,d138,0\H,17,r139,16,a139,14,d139,0\H,17,r140,16,a140,14,d140,0\H,17,r141,16,a141,14,d141,0\H,17,r142,16,a142,14,d142,0\H,17,r143,16,a143,14,d143,0\H,17,r144,16,a144,14,d144,0\H,17,r145,16,a145,14,d145,0\H,17,r146,16,a146,14,d146,0\H,17,r147,16,a147,14,d147,0\H,17,r148,16,a148,14,d148,0\H,17,r149,16,a149,14,d149,0\H,17,r150,16,a150,14,d150,0\H,17,r151,16,a151,14,d151,0\H,17,r152,16,a152,14,d152,0\H,17,r153,16,a153,14,d153,0\H,17,r154,16,a154,14,d154,0\H,17,r155,16,a155,14,d155,0\H,17,r156,16,a156,14,d156,0\H,17,r157,16,a157,14,d157,0\H,17,r158,16,a158,14,d158,0\H,17,r159,16,a159,14,d159,0\H,17,r160,16,a160,14,d160,0\H,17,r161,16,a161,14,d161,0\H,17,r162,16,a162,14,d162,0\H,17,r163,16,a163,14,d163,0\H,17,r164,16,a164,14,d164,0\H,17,r165,16,a165,14,d165,0\H,17,r166,16,a166,14,d166,0\H,17,r167,16,a167,14,d167,0\H,17,r168,16,a168,14,d168,0\H,17,r169,16,a169,14,d169,0\H,17,r170,16,a170,14,d170,0\H,17,r171,16,a171,14,d171,0\H,17,r172,16,a172,14,d172,0\H,17,r173,16,a173,14,d173,0\H,17,r174,16,a174,14,d174,0\H,17,r175,16,a175,14,d175,0\H,17,r176,16,a176,14,d176,0\H,17,r177,16,a177,14,d177,0\H,17,r178,16,a178,14,d178,0\H,17,r179,16,a179,14,d179,0\H,17,r180,16,a180,14,d180,0\H,17,r181,16,a181,14,d181,0\H,17,r182,16,a182,14,d182,0\H,17,r183,16,a183,14,d183,0\H,17,r184,16,a184,14,d184,0\H,17,r185,16,a185,14,d185,0\H,17,r186,16,a186,14,d186,0\H,17,r187,16,a187,14,d187,0\H,17,r188,16,a188,14,d188,0\H,17,r189,16,a189,14,d189,0\H,17,r190,16,a190,14,d190,0\H,17,r191,16,a191,14,d191,0\H,17,r192,16,a192,14,d192,0\H,17,r193,16,a193,14,d193,0\H,17,r194,16,a194,14,d194,0\H,17,r195,16,a195,14,d195,0\H,17,r196,16,a196,14,d196,0\H,17,r197,16,a197,14,d197,0\H,17,r198,16,a198,14,d198,0\H,17,r199,16,a199,14,d199,0\H,17,r200,16,a200,14,d200,0\H,17,r201,16,a201,14,d201,0\H,17,r202,16,a202,14,d202,0\H,17,r203,16,a203,14,d203,0\H,17,r204,16,a204,14,d204,0\H,17,r205,16,a205,14,d205,0\H,17,r206,16,a206,14,d206,0\H,17,r207,16,a207,14,d207,0\H,17,r208,16,a208,14,d208,0\H,17,r209,16,a209,14,d209,0\H,17,r210,16,a210,14,d210,0\H,17,r211,16,a211,14,d211,0\H,17,r212,16,a212,14,d212,0\H,17,r213,16,a213,14,d213,0\H,17,r214,16,a214,14,d214,0\H,17,r215,16,a215,14,d215,0\H,17,r216,16,a216,14,d216,0\H,17,r217,16,a217,14,d217,0\H,17,r218,16,a218,14,d218,0\H,17,r219,16,a219,14,d219,0\H,17,r220,16,a220,14,d220,0\H,17,r221,16,a221,14,d221,0\H,17,r222,16,a222,14,d222,0\H,17,r223,16,a223,14,d223,0\H,17,r224,16,a224,14,d224,0\H,17,r225,16,a225,14,d225,0\H,17,r226,16,a226,14,d226,0\H,17,r227,16,a227,14,d227,0\H,17,r228,16,a228,14,d228,0\H,17,r229,16,a229,14,d229,0\H,17,r230,16,a230,14,d230,0\H,17,r231,16,a231,14,d231,0\H,17,r232,16,a232,14,d232,0\H,17,r233,16,a233,14,d233,0\H,17,r234,16,a234,14,d234,0\H,17,r235,16,a235,14,d235,0\H,17,r236,16,a236,14,d236,0\H,17,r237,16,a237,14,d237,0\H,17,r238,16,a238,14,d238,0\H,17,r239,16,a239,14,d239,0\H,17,r240,16,a240,14,d240,0\H,17,r241,16,a241,14,d241,0\H,17,r242,16,a242,14,d242,0\H,17,r243,16,a243,14,d243,0\H,17,r244,16,a244,14,d244,0\H,17,r245,16,a245,14,d245,0\H,17,r246,16,a246,14,d246,0\H,17,r247,16,a247,14,d247,0\H,17,r248,16,a248,14,d248,0\H,17,r249,16,a249,14,d249,0\H,17,r250,16,a250,14,d250,0\H,17,r251,16,a251,14,d251,0\H,17,r252,16,a252,14,d252,0\H,17,r253,16,a253,14,d253,0\H,17,r254,16,a254,14,d254,0\H,17,r255,16,a255,14,d255,0\H,17,r256,16,a256,14,d256,0\H,17,r257,16,a257,14,d257,0\H,17,r258,16,a258,14,d258,0\H,17,r259,16,a259,14,d259,0\H,17,r260,16,a260,14,d260,0\H,17,r261,16,a261,14,d261,0\H,17,r262,16,a262,14,d262,0\H,17,r263,16,a263,14,d263,0\H,17,r264,16,a264,14,d264,0\H,17,r265,16,a265,14,d265,0\H,17,r266,16,a266,14,d266,0\H,17,r267,16,a267,14,d267,0\H,17,r268,16,a268,14,d268,0\H,17,r269,16,a269,14,d269,0\H,17,r270,16,a270,14,d270,0\H,17,r271,16,a271,14,d271,0\H,17,r272,16,a272,14,d272,0\H,17,r273,16,a273,14,d273,0\H,17,r274,16,a274,14,d274,0\H,17,r275,16,a275,14,d275,0\H,17,r276,16,a276,14,d276,0\H,17,r277,16,a277,14,d277,0\H,17,r278,16,a278,14,d278,0\H,17,r279,16,a279,14,d279,0\H,17,r280,16,a280,14,d280,0\H,17,r281,16,a281,14,d281,0\H,17,r282,16,a282,14,d282,0\H,17,r283,16,a283,14,d283,0\H,17,r284,16,a284,14,d284,0\H,17,r285,16,a285,14,d285,0\H,17,r286,16,a286,14,d286,0\H,17,r287,16,a287,14,d287,0\H,17,r288,16,a288,14,d288,0\H,17,r289,16,a289,14,d289,0\H,17,r290,16,a290,14,d290,0\H,17,r291,16,a291,14,d291,0\H,17,r292,16,a292,14,d292,0\H,17,r293,16,a293,14,d293,0\H,17,r294,16,a294,14,d294,0\H,17,r295,16,a295,14,d295,0\H,17,r296,16,a296,14,d296,0\H,17,r297,16,a297,14,d297,0\H,17,r298,16,a298,14,d298,0\H,17,r299,16,a299,14,d299,0\H,17,r300,16,a300,14,d300,0\H,17,r301,16,a301,14,d301,0\H,17,r302,16,a302,14,d302,0\H,17,r303,16,a303,14,d303,0\H,17,r304,16,a304,14,d304,0\H,17,r305,16,a305,14,d305,0\H,17,r306,16,a306,14,d306,0\H,17,r307,16,a307,14,d307,0\H,17,r308,16,a308,14,d308,0\H,17,r309,16,a309,14,d309,0\H,17,r310,16,a310,14,d310,0\H,17,r311,16,a311,14,d311,0\H,17,r312,16,a312,14,d312,0\H,17,r313,16,a313,14,d313,0\H,17,r314,16,a314,14,d314,0\H,17,r315,16,a315,14,d315,0\H,17,r316,16,a316,14,d316,0\H,17,r317,16,a317,14,d317,0\H,17,r318,16,a318,14,d318,0\H,17,r319,16,a319,14,d319,0\H,17,r320,16,a320,14,d320,0\H,17,r321,16,a321,14,d321,0\H,17,r322,16,a322,14,d322,0\H,17,r323,16,a323,14,d323,0\H,17,r324,16,a324,14,d324,0\H,17,r325,16,a325,14,d325,0\H,17,r326,16,a326,14,d326,0\H,17,r327,16,a327,14,d327,0\H,17,r328,16,a328,14,d328,0\H,17,r329,16,a329,14,d329,0\H,17,r330,16,a330,14,d330,0\H,17,r331,16,a331,14,d331,0\H,17,r332,16,a332,14,d332,0\H,17,r333,16,a333,14,d333,0\H,17,r334,16,a334,14,d334,0\H,17,r335,16,a335,14,d335,0\H,17,r336,16,a336,14,d336,0\H,17,r337,16,a337,14,d337,0\H,17,r338,16,a338,14,d338,0\H,17,r339,16,a339,14,d339,0\H,17,r340,16,a340,14,d340,0\H,17,r341,16,a341,14,d341,0\H,17,r342,16,a342,14,d342,0\H,17,r343,16,a343,14,d343,0\H,17,r344,16,a344,14,d344,0\H,17,r345,16,a345,14,d345,0\H,17,r346,16,a346,14,d346,0\H,17,r347,16,a347,14,d347,0\H,17,r348,16,a348,14,d348,0\H,17,r349,16,a349,14,d349,0\H,17,r350,16,a350,14,d350,0\H,17,r351,16,a351,14,d351,0\H,17,r352,16,a352,14,d352,0\H,17,r353,16,a353,14,d353,0\H,17,r354,16,a354,14,d354,0\H,17,r355,16,a355,14,d355,0\H,17,r356,16,a356,14,d356,0\H,17,r357,16,a357,14,d357,0\H,17,r358,16,a358,14,d358,0\H,17,r359,16,a359,14,d359,0\H,17,r360,16,a360,14,d360,0\H,17,r361,16,a361,14,d361,0\H,17,r362,16,a362,14,d362,0\H,17,r363,16,a363,14,d363,0\H,17,r364,16,a364,14,d364,0\H,17,r365,16,a365,14,d365,0\H,17,r366,16,a366,14,d366,0\H,17,r367,16,a367,14,d367,0\H,17,r368,16,a368,14,d368,0\H,17,r369,16,a369,14,d369,0\H,17,r370,16,a370,14,d370,0\H,17,r371,16,a371,14,d371,0\H,17,r372,16,a372,14,d372,0\H,17,r373,16,a373,14,d373,0\H,17,r374,16,a374,14,d374,0\H,17,r375,16,a375,14,d375,0\H,17,r376,16,a376,14,d376,0\H,17,r377,16,a377,14,d377,0\H,17,r378,16,a378,14,d378,0\H,17,r379,16,a379,14,d379,0\H,17,r380,16,a380,14,d380,0\H,17,r381,16,a381,14,d381,0\H,17,r382,16,a382,14,d382,0\H,17,r383,16,a383,14,d383,0\H,17,r384,16,a384,14,d384,0\H,17,r385,16,a385,14,d385,0\H,17,r386,16,a386,14,d386,0\H,17,r387,16,a387,14,d387,0\H,17,r388,16,a388,14,d388,0\H,17,r389,16,a389,14,d389,0\H,17,r390,16,a390,14,d390,0\H,17,r391,16,a391,14,d391,0\H,17,r392,16,a392,14,d392,0\H,17,r393,16,a393,14,d393,0\H,17,r394,16,a394,14,d394,0\H,17,r395,16,a395,14,d395,0\H,17,r396,16,a396,14,d396,0\H,17,r397,16,a397,14,d397,0\H,17,r398,16,a398,14,d398,0\H,17,r399,16,a399,14,d399,0\H,17,r400,16,a400,14,d400,0\H,17,r401,16,a401,14,d401,0\H,17,r402,16,a402,14,d402,0\H,17,r403,16,a403,14,d403,0\H,17,r404,16,a404,14,d404,0\H,17,r405,16,a405,14,d405,0\H,17,r406,16,a406,14,d406,0\H,17,r407,16,a407,14,d407,0\H,17,r408,16,a408,14,d408,0\H,17,r409,16,a409,14,d409,0\H,17,r410,16,a410,14,d410,0\H,17,r411,16,a411,14,d411,0\H,17,r412,16,a412,14,d412,0\H,17,r413,16,a413,14,d413,0\H,17,r414,16,a414,14,d414,0\H,17,r415,16,a415,14,d415,0\H,17,r416,16,a416,14,d416,0\H,17,r417,16,a417,14,d417,0\H,17,r418,16,a418,14,d418,0\H,17,r419,16,a419,14,d419,0\H,17,r420,16,a420,14,d420,0\H,17,r421,16,a421,14,d421,0\H,17,r422,16,a422,14,d422,0\H,17,r423,16,a423,14,d423,0\H,17,r424,16,a424,14,d424,0\H,17,r425,16,a425,14,d425,0\H,17,r426,16,a426,14,d426,0\H,17,r427,16,a427,14,d427,0\H,17,r428,16,a428,14,d428,0\H,17,r429,16,a429,14,d429,0\H,17,r430,16,a430,14,d430,0\H,17,r431,16,a431,14,d431,0\H,17,r432,16,a432,14,d432,0\H,17,r433,16,a433,14,d433,0\H,17,r434,16,a434,14,d434,0\H,17,r435,16,a435,14,d435,0\H,17,r436,16,a436,14,d436,0\H,17,r437,16,a437,14,d437,0\H,17,r438,16,a438,14,d438,0\H,17,r439,16,a439,14,d439,0\H,17,r440,16,a440,14,d440,0\H,17,r441,16,a441,14,d441,0\H,17,r442,16,a442,14,d442,0\H,17,r443,16,a443,14,d443,0\H,17,r444,16,a444,14,d444,0\H,17,r445,16,a445,14,d445,0\H,17,r446,16,a446,14,d4

Compound 3 (cis-isomer)

Item Value Threshold Converged?
 Maximum Force .000367 .000450 YES
 RMS Force .000091 .000300 YES
 Maximum Displacement .000545 .001800 YES
 RMS Displacement .000144 .001200 YES
 Predicted change in Energy=-3.271771D-08
 Optimization completed.
 -- Stationary point found.

 ! Optimized Parameters !
 ! (Angstroms and Degrees) !

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.081713	.866727	.315264
2	6	0	-1.442423	-.623721	.145022
3	6	0	-.074480	-.773609	-.524599
4	7	0	.058819	.739174	-.658767
5	6	0	1.368252	.661184	.061602
6	6	0	1.156142	-.830079	.407136
7	1	0	-1.831992	1.596142	-.002764
8	1	0	-.750954	1.127878	1.329396
9	1	0	-1.630583	-1.213812	1.047293
10	1	0	-2.263767	-.774951	-.560036
11	1	0	-.006120	-1.365485	-1.444104
12	1	0	2.191488	.827906	-.640142
13	1	0	1.469001	1.369071	.892608
14	1	0	1.954831	-1.514557	.109269
15	1	0	.901694	-1.029426	1.453302

Rotational constants (GHZ): 6.5412446 4.1256583 3.2193197
 Isotopes: C-12,C-12,C-12,N-14,C-12,C-12,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1

Dipole moment (Debye):

X= .0517 Y= -1.1312 Z= 1.4757 Tot= 1.8601

Quadrupole moment (Debye-Ang):

XX= -35.6862 YY= -38.5417 ZZ= -39.1828

XY= -.1828 XZ= -.0850 YZ= 2.5739

Octapole moment (Debye-Ang**2):

XXX= .4997 YYY= -.0788 ZZZ= 2.9863 XYY= .0116

XXY= 1.3286 XXZ= -2.6753 XZZ= -.0449 YZZ= -3.2920

YYZ= 1.9784 XYZ= .4686

Hexadecapole moment (Debye-Ang**3):

XXXX= -335.6354 YYYY= -208.9651 ZZZZ= -110.3501 XXXY= -1.5568

XXXZ= -.2500 YYYYX= -2.4895 YYYZ= 3.9221 ZZZX= -.3888

ZZZY= 4.8058 XXYY= -87.5818 XXZZ= -74.1724 YYZZ= -53.3236

XXYZ= -.2425 YYXZ= -.0260 ZZXY= 1.5898

N-N= 2.479468246639D+02 E-N=-1.076122182981D+03 KE= 2.486066837438D+02

1\1\GINC-ELA\FOpt\RMP2-FC\6-31G(d)\C5H9N1\BELOSTOT\05-Sep-2002\1\# MP
 2/6-31G* GEOM=ALLCHECKPOINT GUESS=CHECKPOINT OPT=Z-MATRIX\1-azabicycl

o220hexane, cis conformation\0,1\C\C,1,r2\C,2,r3,1,a3\N,1,r4,2,a4,3,d
 4,0\C,4,r5,1,a5,2,d5,0\C,3,r6,2,a6,1,d6,0\H,1,r7,2,a7,3,d7,0\H,1,r8,2,
 a8,3,d8,0\H,2,r9,1,a9,3,d9,0\H,2,r10,1,a10,3,d10,0\H,3,r11,2,a11,1,d11
 ,0\H,5,r12,4,a12,1,d12,0\H,5,r13,4,a13,1,d13,0\H,6,r14,3,a14,2,d14,0\H
 ,6,r15,3,a15,2,d15,0\r2=1.5428956\r3=1.53040127\r4=86.21111418\r5=1.5
 0526345\r6=91.36858019\r7=374.18531592\r8=1.49653895\r9=110.84879667\r
 10=257.7123281\r11=1.54458688\r12=116.85905957\r13=77.83038711\r14=1.093666
 69\r15=116.85948294\r16=130.75628153\r17=1.09820985\r18=113.70438468\r19=25
 8.33701856\r20=1.09439787\r21=118.04014986\r22=119.2661208\r23=1.09296979
 \r24=112.36639729\r25=247.65881738\r26=1.09566384\r27=118.41621965\r28=223.99922484\r29=1.09451287\r30=109.97147204\r31=194.51002413\r32=1.0
 962778\r33=114.30793472\r34=-43.07710027\r35=1.09322425\r36=116.142734
 88\r37=142.39876725\r38=1.09496446\r39=113.44409657\r40=15.76761019\r41=

S12

ersion=IBM-RS6000-G98RevA.7\HF=-248.9410519\MP2=-249.7527114\RMSE=3.91
0e-09\RMSF=2.056e-05\Dipole=-0.1596596,0.5729782,0.3255802\PG=C01 [X(C
5H9N1)]\@

ZZZY= 2.9226 XXY= -99.2327 XXZZ= -82.1631 YYZZ= -45.6820
 XXYZ= -3.1556 YYXZ= .0001 ZZXY= .0000
 N-N= 2.454587868476D+02 E-N=-1.070920125276D+03 KE= 2.485293799228D+02
 1\1\GINC-ETROG\FOpt\RMP2-FC\6-31G(d)\C5H9N1\BELOSTOT\05-Sep-2002\0\#
 MP2/6-31G* OPT=(NEWTON, CARTESIAN)\1-azabicyclo220hexane, trans confo
 rmation\0,1\N,0.0074622511,0.0271266547,-0.7064497094\C,0.0128570636,
 0.0476202976,0.7246161332\C,1.5671064075,0.0313791724,0.6539347108\C,1
 .2696170012,-0.7640866963,-0.678229538\C,-1.4815802503,-0.0155889037,-
 0.6785472015\C,-1.3353083692,0.8211290304,0.6535257302\H,-0.2581003763
 ,-0.9479433824,1.1548573653\H,2.0035045972,1.0074139307,0.4344659529\H
 ,2.1196585752,-0.4849099588,1.4446028635\H,1.137917107,-1.8387704312,-
 0.4684359488\H,1.9274987027,-0.6206340588,-1.5404640836\H,-1.975922755
 2,0.4412841842,-1.5409541716\H,-1.9125542696,-1.0088365129,-0.46870669
 86\H,-2.0734605423,0.6561068452,1.4440488963\H,-1.2169279138,1.8836853
 983,0.4339347819\Version=IBM-RS6000-G98RevA.7\HF=-248.8792926\MP2=-24
 9.7003999\RMSD=3.557e-09\RMSF=1.713e-05\Dipole=-0.0570751,-0.2098058,0
 .1243385\PG=C01 [X(C5H9N1)]\@

Dipole moment (Debye):
X= .0000 Y= -.1399 Z= -.0801 Tot= .1612
Quadrupole moment (Debye-Ang):
XX= -35.6865 YY= -38.3410 ZZ= -37.9597
XY= .0000 XZ= .0000 YZ= -.1537
Octapole moment (Debye-Ang**2):
XXX= .0000 YYY= 2.5729 ZZZ= -1.8062 XYY= .0000

S16

XXY= 2.0660 XXZ= -.2900 XZZ= .0000 YZZ= -.0171

YYZ= -1.1332 XYZ= .0000

Hexadecapole moment (Debye-Ang**3):

XXXX= -432.5431 YYYY= -207.0962 ZZZZ= -83.4142 XXXY= .0000

XXXZ= .0000 YYYX= .0000 YYYZ= -2.4320 ZZZX= .0000

ZZZY= 1.5779 XXYY= -101.9965 XXZZ= -83.3382 YYZZ= -46.7104

XXYZ= -2.8504 YYXZ= .0000 ZZXY= .0000

N-N= 2.450693670139D+02 E-N=-1.070233078272D+03 KE= 2.485159709530D+02

Exact polarizability: 66.074 6.897 52.611 -.448 1.064 53.547

Approx polarizability: 52.940 .000 45.941 .000 -2.246 47.487

Rotating electric field derivatives to standard orientation.

Rotating nuclear coordinate derivatives to standard orientation.

Full mass-weighted force constant matrix:

Low frequencies --- -306.0064 -.0012 -.0011 -.0009 4.0668 5.2537

Low frequencies --- 6.6765 244.9346 367.2016

***** 1 imaginary frequencies (negative Signs) *****

Harmonic frequencies (cm**-1), IR intensities (KM/Mole),

Raman scattering activities (A**4/AMU), Raman depolarization ratios,

reduced masses (AMU), force constants (mDyne/A) and normal coordinates:

1 ?A			2 ?A			3 ?A			
Frequencies --	-306.0063		244.9346		367.2016				
Red. masses --	3.5346		1.7523		2.2671				
Frc consts --	.1950		.0619		.1801				
IR Inten --	13.9418		.6520		1.7407				
Raman Activ --	.0000		.0000		.0000				
Depolar --	.0000		.0000		.0000				
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 7	.00	.05	.37	-.01	.00	.00	.00	.11	-.04
2 6	.00	-.03	.09	-.03	.00	.00	.00	.14	.11
3 6	-.05	.00	-.06	.02	-.02	.12	-.15	-.05	-.04
4 6	-.01	.00	-.14	-.01	.01	-.13	.06	-.06	.02
5 6	.01	.00	-.14	-.01	-.01	.13	-.06	-.06	.02
6 6	.05	.00	-.06	.02	.02	-.12	.15	-.05	-.04
7 1	.00	-.32	.04	-.15	.00	.00	.00	.29	.13
8 1	.01	.02	-.11	-.04	.11	.32	-.10	-.20	-.25
9 1	-.14	-.06	-.05	.16	-.23	.18	-.44	.03	-.07
10 1	-.21	-.06	-.31	-.10	-.13	-.30	.18	-.07	.08
11 1	.27	.10	-.30	.11	.20	-.25	.03	-.18	.06
12 1	-.27	.10	-.30	.11	-.20	.25	-.03	-.18	.06
13 1	.21	-.06	-.31	-.10	.13	.30	-.18	-.07	.08
14 1	.14	-.06	-.05	.16	.23	-.18	.44	.03	-.07
15 1	-.01	.02	-.11	-.04	-.11	-.32	.10	-.20	-.25

4 ?A			5 ?A			6 ?A			
Frequencies --	535.0598		700.3369		730.5677				
Red. masses --	2.3712		1.7955		2.9695				
Frc consts --	.4000		.5189		.9338				
IR Inten --	3.8883		.3468		1.1543				
Raman Activ --	.0000		.0000		.0000				
Depolar --	.0000		.0000		.0000				
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 7	.00	.17	.06	.08	.00	.00	.00	-.03	-.02
2 6	.00	.09	-.18	-.06	.00	.00	.00	-.01	.12
3 6	.02	-.05	.03	-.09	.06	.06	.18	.08	-.01
4 6	.12	-.06	.00	.09	.08	.02	.20	-.07	-.01
5 6	-.12	-.06	.00	.09	-.08	-.02	-.20	-.07	-.01
6 6	-.02	-.05	.03	-.09	-.06	-.06	-.18	.08	-.01
7 1	.00	-.08	-.20	-.23	.00	.00	.00	.01	.12
8 1	-.22	-.03	.33	-.02	-.15	-.23	.39	.08	-.28
9 1	.36	-.18	.07	-.32	.30	-.01	-.06	.21	-.05
10 1	.18	-.12	-.01	.03	-.11	-.16	.20	-.15	-.06
11 1	.19	-.11	-.02	.16	.31	-.09	.22	-.02	-.04
12 1	-.19	-.11	-.02	.16	-.31	.09	-.22	-.02	-.04
13 1	-.18	-.12	-.01	.03	.11	.16	-.20	-.15	-.06
14 1	-.36	-.18	.07	-.32	-.30	.01	.06	.21	-.05
15 1	.22	-.03	.33	-.02	.15	.23	-.39	.08	-.28

7 ?A			8 ?A			9 ?A		
Frequencies --	815.3419		860.5738		908.0459			
Red. masses --	1.4834		3.0598		1.7080			

S17

Frc consts --	.5810	1.3351	.8298
IR Inten --	1.2744	.7226	.1170
Raman Activ --	.0000	.0000	.0000
Depolar --	.0000	.0000	.0000

Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 7	.00	-.04	-.03	-.04	.00	.00	.06	.00	.00
2 6	.00	-.07	-.07	-.11	.00	.00	-.05	.00	.00
3 6	-.06	-.01	.05	.00	.22	.01	-.09	.05	-.04
4 6	.06	.06	.04	.05	-.18	-.03	.08	.09	-.03
5 6	-.06	.06	.04	.05	.18	.03	.08	-.09	.03
6 6	.06	-.01	.05	.00	-.22	-.01	-.09	-.05	.04
7 1	.00	-.14	-.08	-.17	.00	.00	-.04	.00	.00
8 1	-.15	-.26	-.10	.16	.42	.00	-.20	.20	.26
9 1	-.05	.29	-.03	-.01	.14	.03	.07	-.29	.05
10 1	.01	-.24	-.21	.16	-.25	-.01	.08	.35	.17
11 1	.10	.40	-.10	.08	-.27	-.02	.08	-.23	.08
12 1	-.10	.40	-.10	.08	.27	.02	.08	.23	-.08
13 1	-.01	-.24	-.21	.16	.25	.01	.08	-.35	-.17
14 1	.05	.29	-.03	-.01	-.14	-.03	.07	.29	-.05
15 1	.15	-.26	-.10	.16	-.42	.00	-.20	-.20	-.26

10

11

12

?A

?A

?A

Frequencies --	929.7624	943.8211	995.7903
Red. masses --	3.0252	2.2357	1.1841
Frc consts --	1.5408	1.1734	.6918
IR Inten --	.2768	4.2166	3.6335
Raman Activ --	.0000	.0000	.0000
Depolar --	.0000	.0000	.0000

Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 7	.00	-.06	-.03	.00	-.10	-.03	.01	.00	.00
2 6	.00	-.12	-.01	.00	-.08	.07	.00	.00	.00
3 6	-.16	.21	.02	-.05	-.03	-.03	.04	-.02	.06
4 6	.01	-.11	-.02	.15	.13	-.01	-.02	.01	-.04
5 6	-.01	-.11	-.02	-.15	.13	-.01	-.02	-.01	.04
6 6	.16	.21	.02	.05	-.03	-.03	.04	.02	-.06
7 1	.00	-.25	-.03	.00	-.21	.04	-.31	.00	.00
8 1	-.16	.43	.22	-.12	.06	.15	.29	.05	-.18
9 1	.04	.04	.07	-.05	-.35	.05	-.43	-.17	.08
10 1	.16	-.20	.00	-.01	.42	.12	-.01	.22	.12
11 1	.03	-.21	.01	.22	-.13	.05	-.05	-.19	.04
12 1	-.03	-.21	.01	-.22	-.13	.05	-.05	.19	-.04
13 1	-.16	-.20	.00	.01	.42	.12	-.01	-.22	-.12
14 1	-.04	.04	.07	.05	-.35	.05	-.43	.17	-.08
15 1	.16	.43	.22	.12	.06	.15	.29	-.05	.18

13

14

15

?A

?A

?A

Frequencies --	1069.6811	1105.5348	1159.4426
Red. masses --	2.5361	1.2852	1.2244
Frc consts --	1.7097	.9254	.9698
IR Inten --	7.2971	2.3926	18.2974
Raman Activ --	.0000	.0000	.0000
Depolar --	.0000	.0000	.0000

Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 7	-.07	.00	.00	.00	.05	.04	.01	.00	.00
2 6	.30	.00	.00	.00	-.07	.00	.08	.00	.00
3 6	-.10	.05	.08	.01	-.02	.03	-.01	.02	.01
4 6	.00	-.01	-.04	.01	.04	-.07	-.02	-.03	.07
5 6	.00	.01	.04	-.01	.04	-.07	-.02	.03	-.07
6 6	-.10	-.05	-.08	-.01	-.02	.03	-.01	-.02	-.01
7 1	.49	.00	.00	.00	-.30	-.03	.11	.00	.00
8 1	-.19	-.05	.08	.03	-.07	-.05	-.06	.00	.04
9 1	-.29	-.04	.10	-.05	.04	.01	-.12	-.06	.03
10 1	.32	-.15	.03	.46	.00	.14	-.43	.07	-.07
11 1	-.19	-.09	.06	-.43	.03	.12	.48	-.15	-.10
12 1	-.19	.09	-.06	.43	.03	.12	.48	.15	.10
13 1	.32	.15	-.03	-.46	.00	.14	-.43	-.07	.07
14 1	-.29	.04	-.10	.05	.04	.01	-.12	.06	-.03
15 1	-.19	.05	-.08	-.03	-.07	-.05	-.06	.00	-.04

16

17

18

?A

?A

?A

Frequencies --	1173.5104	1207.8291	1210.5639
----------------	-----------	-----------	-----------

S18

Red. masses --	1.7391	1.5939	1.2776
Frc consts --	1.4111	1.3700	1.1031
IR Inten --	2.1983	14.8347	.0132
Raman Activ --	.0000	.0000	.0000
Depolar --	.0000	.0000	.0000
Atom AN	X Y Z	X Y Z	X Y Z
1 7	.00 .02 -.02	.00 .12 -.04	-.02 .00 .00
2 6	.00 .00 .14	.00 -.11 -.08	-.03 .00 .00
3 6	-.02 -.04 -.13	-.02 -.05 .04	.04 .03 .05
4 6	-.01 .02 .06	-.03 .04 .04	.01 -.03 -.08
5 6	.01 .02 .06	.03 .04 .04	.01 .03 .08
6 6	.02 -.04 -.13	.02 -.05 .04	.04 -.03 -.05
7 1	.00 -.02 .13	.00 -.11 -.10	.00 .00 .00
8 1	.02 .23 .11	.41 .33 -.13	-.27 -.41 .00
9 1	.34 -.15 -.09	-.24 -.19 .07	.10 .31 -.02
10 1	.19 -.32 -.09	.04 -.14 -.05	-.10 .28 .09
11 1	-.11 .30 .02	.22 -.04 -.04	-.03 -.21 .00
12 1	.11 .30 .02	-.22 -.04 -.04	-.03 .21 .00
13 1	-.19 -.32 -.09	-.04 -.14 -.05	-.10 -.28 -.09
14 1	-.34 -.15 -.09	.24 -.19 .07	.10 -.31 .02
15 1	-.02 .23 .11	-.41 .33 -.13	-.27 .41 .00
	19	20	21
	?A	?A	?A
Frequencies --	1249.0015	1257.4682	1269.3298
Red. masses --	1.4969	1.3620	1.2586
Frc consts --	1.3759	1.2689	1.1948
IR Inten --	9.1090	1.1050	6.9144
Raman Activ --	.0000	.0000	.0000
Depolar --	.0000	.0000	.0000
Atom AN	X Y Z	X Y Z	X Y Z
1 7	-.08 .00 .00	.00 .08 -.06	.00 -.05 .07
2 6	-.03 .00 .00	.00 -.03 .08	.00 -.07 -.05
3 6	.09 .07 -.06	-.05 -.05 .03	-.03 -.02 .01
4 6	.04 -.01 .03	.00 .00 -.03	.01 .04 -.02
5 6	.04 .01 -.03	.00 .00 -.03	-.01 .04 -.02
6 6	.09 -.07 .06	.05 -.05 .03	.03 -.02 .01
7 1	-.13 .00 .00	.00 -.31 .04	.00 .85 .09
8 1	-.29 -.28 .08	.10 .04 -.05	.07 .09 -.02
9 1	-.28 -.41 .05	.38 .43 -.08	.17 .16 -.03
10 1	.00 -.07 -.03	-.13 .18 .04	.19 -.02 .02
11 1	-.08 .20 .01	.11 -.16 -.03	.06 -.12 .01
12 1	-.08 -.20 -.01	-.11 -.16 -.03	-.06 -.12 .01
13 1	.00 .07 .03	.13 .18 .04	-.19 -.02 .02
14 1	-.28 .41 -.05	-.38 .43 -.08	-.17 .16 -.03
15 1	-.29 .28 -.08	-.10 .04 -.05	-.07 .09 -.02
	22	23	24
	?A	?A	?A
Frequencies --	1284.7291	1295.2719	1334.0572
Red. masses --	1.8265	1.5949	3.0049
Frc consts --	1.7762	1.5765	3.1509
IR Inten --	24.1676	50.5572	74.6967
Raman Activ --	.0000	.0000	.0000
Depolar --	.0000	.0000	.0000
Atom AN	X Y Z	X Y Z	X Y Z
1 7	.00 -.10 .05	-.09 .00 .00	.34 .00 .00
2 6	.00 .16 -.08	.01 .00 .00	.00 .00 .00
3 6	-.07 -.05 .02	-.04 -.02 .01	-.01 .06 -.01
4 6	.07 -.04 .00	.12 -.07 .00	-.11 -.09 -.01
5 6	-.07 -.04 .00	.12 .07 .00	-.11 .09 .01
6 6	.07 -.05 .02	-.04 .02 -.01	-.01 -.06 .01
7 1	.00 -.09 -.10	.22 .00 .00	.18 .00 .00
8 1	.32 .39 -.05	.13 .16 -.03	-.15 .02 .12
9 1	.00 .08 -.01	.01 .01 .01	-.17 -.07 .02
10 1	-.14 .16 .03	-.36 .32 .04	-.26 .07 .02
11 1	-.29 .25 .05	-.25 .32 .02	-.43 .27 .03
12 1	.29 .25 .05	-.25 -.32 -.02	-.43 -.27 -.03
13 1	.14 .16 .03	-.36 -.32 -.04	-.26 -.07 -.02
14 1	.00 .08 -.01	.01 -.01 -.01	-.17 .07 -.02
15 1	-.32 .39 -.05	.13 -.16 .03	-.15 -.02 -.12
	25	26	27
	?A	?A	?A

S19

Frequencies --	1360.2291	1414.9797	1528.2133
Red. masses --	1.8075	1.3097	1.1212
Frc consts --	1.9704	1.5450	1.5428
IR Inten --	7.5991	18.3824	.0384
Raman Activ --	.0000	.0000	.0000
Depolar --	.0000	.0000	.0000

Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 7	.00	.14	-.01	.00	.00	.00	-.02	.00	.00
2 6	.00	-.17	.01	-.15	.00	.00	-.01	.00	.00
3 6	-.01	.02	-.01	.03	.00	.04	.04	-.05	-.02
4 6	.05	-.08	.00	.00	.02	.00	.00	.00	.00
5 6	-.05	-.08	.00	.00	-.02	.00	.00	.00	.00
6 6	.01	.02	-.01	.03	.00	-.04	.04	.05	.02
7 1	.00	.39	.08	.93	.00	.00	-.01	.00	.00
8 1	-.04	-.03	-.02	.08	-.02	-.05	-.12	.22	.42
9 1	.02	-.11	.03	-.13	-.07	.05	-.35	.33	-.12
10 1	-.29	.30	.09	.08	-.02	.01	.05	.02	.04
11 1	-.23	.37	-.02	.09	-.04	-.01	.04	.04	-.03
12 1	.23	.37	-.02	.09	.04	.01	.04	-.04	.03
13 1	.29	.30	.09	.08	.02	-.01	.05	-.02	-.04
14 1	-.02	-.11	.03	-.13	.07	-.05	-.35	-.33	.12
15 1	.04	-.03	-.02	.08	.02	.05	-.12	-.22	-.42

28

?A

29

?A

30

?A

Frequencies --	1532.8677	1572.3428	1587.0790
Red. masses --	1.1150	1.1018	1.1164
Frc consts --	1.5437	1.6048	1.6568
IR Inten --	2.8272	17.3453	1.9555
Raman Activ --	.0000	.0000	.0000
Depolar --	.0000	.0000	.0000

Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 7	.00	.01	.00	-.01	.00	.00	.00	-.03	.00
2 6	.00	-.02	.00	.01	.00	.00	.00	.03	.00
3 6	.04	-.05	-.03	-.01	.01	.00	-.01	.01	.00
4 6	.00	-.01	.00	-.04	-.05	-.01	-.05	-.04	.00
5 6	.00	-.01	.00	-.04	.05	.01	.05	-.04	.00
6 6	-.04	-.05	-.03	-.01	-.01	.00	.01	.01	.00
7 1	.00	.01	.01	-.03	.00	.00	.00	-.04	-.02
8 1	-.13	.21	.42	.00	-.02	-.05	.02	-.03	-.08
9 1	-.35	.32	-.12	.05	-.03	.01	.06	-.05	.02
10 1	.05	.05	.06	.28	.22	.34	.30	.19	.34
11 1	.05	.07	-.05	.28	.33	-.24	.31	.30	-.24
12 1	-.05	.07	-.05	.28	-.33	.24	-.31	.30	-.24
13 1	-.05	.05	.06	.28	-.22	-.34	-.30	.19	.34
14 1	.35	.32	-.12	.05	.03	-.01	-.06	-.05	.02
15 1	.13	.21	.42	.00	.02	.05	-.02	-.03	-.08

31

?A

32

?A

33

?A

Frequencies --	2897.0144	3007.2173	3015.0676
Red. masses --	1.0819	1.0684	1.0688
Frc consts --	5.3496	5.6925	5.7244
IR Inten --	129.2145	142.8214	108.1080
Raman Activ --	.0000	.0000	.0000
Depolar --	.0000	.0000	.0000

Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 7	.00	.00	.00	.00	.00	.00	.00	.00	.00
2 6	.00	.01	-.08	.00	.00	.00	.00	.00	.00
3 6	.00	.00	.00	.00	.00	.00	.00	.00	.00
4 6	.00	.00	.00	.02	.02	.04	-.02	-.02	-.04
5 6	.00	.00	.00	.02	-.02	-.04	.02	-.02	-.04
6 6	.00	.00	.00	.00	.00	.00	.00	.00	.00
7 1	.00	-.14	.98	.00	.00	.00	.00	-.02	.05
8 1	-.01	.01	-.02	.01	-.01	.01	-.02	.02	-.02
9 1	.00	-.01	-.01	.00	.00	.01	.00	.00	.00
10 1	.00	.00	.01	-.06	-.08	.13	.05	.07	-.12
11 1	-.01	-.01	-.04	-.24	-.19	-.61	.25	.19	.61
12 1	.01	-.01	-.04	-.24	.19	.61	-.25	.19	.61
13 1	.00	.00	.01	-.06	.08	-.13	-.05	.07	-.12
14 1	.00	-.01	-.01	.00	.00	-.01	.00	.00	.00
15 1	.01	.01	-.02	.01	.01	-.01	.02	.02	-.02

34

35

36

S20

	?A	?A	?A
Frequencies --	3119.4379	3120.3767	3138.9790
Red. masses --	1.0596	1.0596	1.0970
Frc consts --	6.0748	6.0786	6.3683
IR Inten --	53.2757	40.7177	30.2857
Raman Activ --	.0000	.0000	.0000
Depolar --	.0000	.0000	.0000

Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 7	.00	.00	.00	.00	.00	.00	.00	.00	.00
2 6	.00	.00	.00	.00	.00	.00	.00	.00	.00
3 6	.03	-.03	-.01	-.03	.03	.01	.00	.00	.01
4 6	.00	.00	.00	.00	.00	-.01	.02	.03	-.05
5 6	.00	.00	.00	.00	.00	-.01	.02	-.03	.05
6 6	.03	.03	.01	.03	.03	.01	.00	.00	-.01
7 1	.00	.00	.00	.00	.00	.02	.00	.00	.00
8 1	-.39	.30	-.32	.38	-.30	.31	-.05	.04	-.04
9 1	.00	.09	.38	.01	-.09	-.39	.00	.00	-.02
10 1	.02	.02	-.03	-.03	-.04	.05	-.27	-.37	.51
11 1	-.01	-.01	-.02	.02	.01	.03	.06	.05	.12
12 1	-.01	.01	.02	-.02	.01	.03	.06	-.05	-.12
13 1	.02	-.02	.03	.03	-.04	.05	-.27	.37	-.51
14 1	.00	-.09	-.38	-.01	-.09	-.39	.00	.00	.02
15 1	-.39	-.30	.32	-.38	-.30	.31	-.05	-.04	.04

	37 ?A	38 ?A	39 ?A
Frequencies --	3140.1626	3200.5342	3201.5759
Red. masses --	1.0954	1.1089	1.1087
Frc consts --	6.3640	6.6923	6.6955
IR Inten --	60.7356	7.2383	45.6574
Raman Activ --	.0000	.0000	.0000
Depolar --	.0000	.0000	.0000

Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 7	.00	.00	.00	.00	.00	.00	.00	.00	.00
2 6	.00	.00	.00	.00	.00	.00	.00	.00	.00
3 6	-.01	.01	.00	-.02	.00	-.06	.02	.00	.06
4 6	-.02	-.03	.05	.00	.00	-.01	.00	.00	.01
5 6	.02	-.03	.05	.00	.00	.01	.00	.00	.01
6 6	.01	.01	.00	-.02	.00	.06	-.02	.00	.06
7 1	.00	.00	.01	.00	.00	.00	.00	.01	-.04
8 1	.06	-.05	.05	.26	-.20	.20	-.26	.20	-.20
9 1	.00	.00	.00	-.02	.15	.57	.02	-.14	-.56
10 1	.27	.37	-.51	-.02	-.03	.04	.02	.03	-.03
11 1	-.05	-.05	-.11	.01	.01	.03	-.01	-.01	-.03
12 1	.05	-.05	-.11	.01	-.01	-.03	.01	-.01	-.03
13 1	-.27	.37	-.51	-.02	.03	-.04	-.02	.03	-.03
14 1	.00	.00	.00	-.02	-.15	-.57	-.02	-.14	-.56
15 1	-.06	-.05	.05	.26	.20	-.20	.26	.20	-.20

 - Thermochemistry -

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Atom 1 has atomic number 7 and mass 14.00307

Atom 2 has atomic number 6 and mass 12.00000

Atom 3 has atomic number 6 and mass 12.00000

Atom 4 has atomic number 6 and mass 12.00000

Atom 5 has atomic number 6 and mass 12.00000

Atom 6 has atomic number 6 and mass 12.00000

Atom 7 has atomic number 1 and mass 1.00783

Atom 8 has atomic number 1 and mass 1.00783

Atom 9 has atomic number 1 and mass 1.00783

Atom 10 has atomic number 1 and mass 1.00783

Atom 11 has atomic number 1 and mass 1.00783

Atom 12 has atomic number 1 and mass 1.00783

Atom 13 has atomic number 1 and mass 1.00783

Atom 14 has atomic number 1 and mass 1.00783

Atom 15 has atomic number 1 and mass 1.00783

Molecular mass: 83.07350 amu.

Principal axes and moments of inertia in atomic units:

	1	2	3
EIGENVALUES --	234.81204	506.76935	661.76770

X 1.00000 .00000 .00000
 Y .00000 1.00000 .00296
 Z .00000 -.00296 1.00000
 THIS MOLECULE IS AN ASYMMETRIC TOP.
 ROTATIONAL SYMMETRY NUMBER 1.
 ROTATIONAL TEMPERATURES (KELVIN) .36886 .17091 .13088
 ROTATIONAL CONSTANTS (GHZ) 7.68590 3.56127 2.72715
 1 IMAGINARY FREQUENCIES IGNORED.
 Zero-point vibrational energy 355793.0 (Joules/Mol)
 85.03656 (Kcal/Mol)
 WARNING-- EXPLICIT CONSIDERATION OF 3 DEGREES OF FREEDOM AS
 VIBRATIONS MAY CAUSE SIGNIFICANT ERROR
 VIBRATIONAL TEMPERATURES: 352.40 528.32 769.83 1007.62 1051.12
 (KELVIN) 1173.09 1238.17 1306.47 1337.71 1357.94
 1432.71 1539.02 1590.61 1668.17 1688.41
 1737.79 1741.72 1797.02 1809.21 1826.27
 1848.43 1863.60 1919.40 1957.06 2035.83
 2198.75 2205.44 2262.24 2283.44 4168.13
 4326.69 4337.98 4488.15 4489.50 4516.26
 4517.97 4604.83 4606.33

Zero-point correction= .135514 (Hartree/Particle)
 Thermal correction to Energy= .140144
 Thermal correction to Enthalpy= .141088
 Thermal correction to Gibbs Free Energy= .107622
 Sum of electronic and zero-point Energies= -249.560661
 Sum of electronic and thermal Energies= -249.556031
 Sum of electronic and thermal Enthalpies= -249.555087
 Sum of electronic and thermal Free Energies= -249.588554

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	87.942	17.856	70.436
ELECTRONIC	.000	.000	.000
TRANSLATIONAL	.889	2.981	39.165
ROTATIONAL	.889	2.981	25.868
VIBRATIONAL	86.164	11.894	5.402
VIBRATION 1	.660	1.771	1.767
VIBRATION 2	.740	1.540	1.091
VIBRATION 3	.890	1.172	.576
Q	LOG10(Q)	LN(Q)	
TOTAL BOT	.314521D-49	-49.502351	-113.983375
TOTAL V=0	.675333D+13	12.829518	29.541056
VIB (BOT)	.105203D-61	-61.977972	-142.709555
VIB (BOT) 1	.798732D+00	-.097599	-.224730
VIB (BOT) 2	.496749D+00	-.303863	-.699671
VIB (BOT) 3	.297491D+00	-.526527	-1.212373
VIB (V=0)	.225890D+01	.353896	.814876
VIB (V=0) 1	.144232D+01	.159063	.366255
VIB (V=0) 2	.120481D+01	.080919	.186323
VIB (V=0) 3	.108181D+01	.034150	.078634
ELECTRONIC	.100000D+01	.000000	.000000
TRANSLATIONAL	.297615D+08	7.473654	17.208725
ROTATIONAL	.100454D+06	5.001967	11.517456

**** Axes restored to original set ****

Center Number	Atomic Number	Forces (Hartrees/Bohr)		
		X	Y	Z
1	7	-.000000462	.000000849	-.000125677
2	6	.000027030	-.000064078	.000069690
3	6	.000003990	-.000004192	.000009371
4	6	-.000001539	-.000015962	-.000007369
5	6	.000012544	-.000010091	-.000007352
6	6	.000000244	-.000005774	.000009317
7	1	-.000003414	.000008080	-.000017088
8	1	-.000027108	-.000017232	-.000011800
9	1	.000002578	.000023609	.000005323
10	1	-.000041376	.000020916	.000052591
11	1	-.000009290	-.000005331	-.000011576
12	1	.000010330	.000002923	-.000011582

S22

13	1	.000013932	.000044276	.000052645
14	1	-.000018696	.000014648	.000005309
15	1	.000031237	.000007361	-.000011801

Cartesian Forces: Max .000125677 RMS .000030033
1\1\GINC-ESHEL\Freq\RMP2-FC\6-31G(d)\C5H9N1\BELOSTOT\19-Sep-2002\0\#\n
MP2/6-31G* OPT=(NEWTON, CARTESIAN, TS, CALCALL)\1-azabicyclo220hexane
, RINI TS\0,1\N,-0.048675573,0.1154939655,-0.6453681161\C,-0.07285272
03,0.1729357431,0.7665932014\C,1.4868883465,0.2336683781,0.7091952288\
C,1.2647195222,0.7461187909,-0.7711139934\C,-1.4173388306,-0.383973809
7,-0.7710645056\C,-1.2057331447,-0.900874386,0.7092452931\H,-0.4709090
977,1.1176664947,1.2057508154\H,2.0066186314,0.9012974023,1.4055364341
\H,1.9476265003,-0.7574164036,0.7081509147\H,1.9151752369,0.3439290945
, -1.5558604069\H,1.262189773,1.8498201234,-0.830607425\H,-2.2054380857
,0.3887255538,-0.8305439078\H,-1.5838524609,-1.1303963904,-1.555795611
5\H,-0.8182702901,-1.9228338962,0.70820304\H,-2.0465102372,-0.80649803
65,1.405611614\Version=IBM-RS6000-G98RevA.7\HF=-248.880651\MP2=-249.6
961755\RMSE=4.938e-09\RMSE=3.003e-05\Dipole=0.0257804,-0.0611851,0.003
3841\

Compound 3 (ring inversion transition state)

Item Value Threshold Converged?
 Maximum Force .000013 .000450 YES
 RMS Force .000006 .000300 YES
 Maximum Displacement .001101 .001800 YES
 RMS Displacement .000584 .001200 YES
 Predicted change in Energy= 1.452293D-09
 Optimization completed.
 -- Stationary point found.
 Grad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	-.325990	.519709	-.777249
2	6	0	-.302028	.481054	.745204
3	6	0	1.235743	.501100	.767267
4	6	0	1.172625	.461976	-.777010
5	6	0	-.926228	-.854645	-.777460
6	6	0	-.988344	-.895248	.766820
7	1	0	-.812263	1.293523	1.274198
8	1	0	1.663633	1.420823	1.174264
9	1	0	1.710940	-.352525	1.261110
10	1	0	1.574759	-.443200	-1.248373
11	1	0	1.608549	1.332138	-1.277067
12	1	0	-1.899628	-.868028	-1.277037
13	1	0	-.286591	-1.610413	-1.249575
14	1	0	-.425655	-1.694341	1.259974
15	1	0	-2.002416	-.881350	1.174327

Stoichiometry C5H9N
 Framework group C1[X(C5H9N)]
 Deg. of freedom 39
 Full point group C1 NOp 1
 Largest Abelian subgroup C1 NOp 1
 Largest concise Abelian subgroup C1 NOp 1
 Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	.000115	.741867	-.655832
2	6	0	-.000141	-.775688	-.525614
3	6	0	-1.313316	-.752690	.274803
4	6	0	-1.238543	.789142	.188368
5	6	0	1.239092	.788738	.187893
6	6	0	1.312774	-.753091	.275290
7	1	0	-.000028	-1.357305	-1.454056
8	1	0	-2.164779	-1.189497	-.253247
9	1	0	-1.262216	-1.191435	1.276432
10	1	0	-1.097833	1.314343	1.141050
11	1	0	-2.070164	1.260550	-.344032
12	1	0	2.070855	1.259071	-.345230
13	1	0	1.099213	1.314767	1.140229
14	1	0	1.260780	-1.191097	1.277196
15	1	0	2.164182	-1.190934	-.251963

Rotational constants (GHZ): 6.4736601 4.1350715 3.1641874
 Isotopes: N-14,C-12,C-12,C-12,C-12,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1
 Rotating electric field derivatives to standard orientation.
 Rotating nuclear coordinate derivatives to standard orientation.
 Full mass-weighted force constant matrix:
 Low frequencies --- -93.4985 -.0005 -.0002 .0002 2.0367 2.5339
 Low frequencies --- 3.1894 322.5323 422.2162
 ***** 1 imaginary frequencies (negative Signs) *****
 Harmonic frequencies (cm**-1), IR intensities (KM/Mole),
 Raman scattering activities (A**4/AMU), Raman depolarization ratios,

S24

reduced masses (AMU), force constants (mDyne/A) and normal coordinates:

1				2				3				
?A				?A				?A				
Frequencies --	-93.4984						322.5323			422.2162		
Red. masses --	1.7883						1.7886			2.4694		
Frc consts --	.0092						.1096			.2594		
IR Inten --	.6266						.5543			1.3446		
Raman Activ --	.0000						.0000			.0000		
Depolar --	.0000						.0000			.0000		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z	X	Y	Z
1 7	.03	.00	.00	.00	-.09	-.01	.00	.02	.18			
2 6	-.01	.00	.00	.00	-.07	.12	.00	.05	.08			
3 6	.05	.04	.11	-.12	.04	-.06	-.09	-.02	-.03			
4 6	-.05	.04	-.12	.02	.03	.01	-.17	-.01	-.07			
5 6	-.05	-.04	.12	-.02	.03	.01	.17	-.01	-.07			
6 6	.05	-.04	-.11	.12	.04	-.06	.09	-.02	-.03			
7 1	-.13	.00	.00	.00	-.14	.16	.00	.15	.01			
8 1	.02	-.11	.29	-.02	.17	-.33	.00	-.14	-.08			
9 1	.20	.21	.18	-.45	-.04	-.08	-.14	.05	.00			
10 1	-.20	.23	-.21	.15	-.08	.06	-.48	.06	-.06			
11 1	-.03	-.14	-.30	.05	.20	.12	-.05	-.11	-.35			
12 1	-.03	.14	.30	-.05	.20	.12	.05	-.12	-.35			
13 1	-.20	-.23	.21	-.15	-.08	.06	.48	.06	-.06			
14 1	.20	-.21	-.18	.45	-.04	-.07	.14	.05	.00			
15 1	.02	.11	-.29	.03	.17	-.33	.00	-.14	-.08			
4				5				6				
?A				?A				?A				
Frequencies --	686.2887						736.2838			781.1417		
Red. masses --	4.3968						2.1291			1.1088		
Frc consts --	1.2201						.6800			.3986		
IR Inten --	.0288						6.6656			.7103		
Raman Activ --	.0000						.0000			.0000		
Depolar --	.0000						.0000			.0000		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z	X	Y	Z
1 7	.19	.00	.00	.00	.16	-.15	.00	.00	.00			
2 6	-.18	.00	.00	.00	.05	.13	.01	.00	.00			
3 6	-.18	-.16	.06	.08	-.04	.03	-.01	.02	-.05			
4 6	.16	-.16	-.06	-.04	-.05	.02	-.02	.00	-.03			
5 6	.16	.16	.06	.04	-.05	.02	-.02	.00	.03			
6 6	-.18	.16	-.06	-.08	-.04	.03	-.01	-.02	.05			
7 1	-.13	.00	.00	.00	-.13	.25	.07	.00	.00			
8 1	-.32	-.13	.27	.24	.10	-.34	-.03	-.28	.22			
9 1	.04	-.07	.09	-.22	-.28	-.06	.23	.31	.06			
10 1	.05	-.16	-.05	-.07	.07	-.05	.11	-.30	.12			
11 1	.25	-.13	-.16	-.15	-.26	.01	.02	.28	.15			
12 1	.25	.13	.16	.15	-.26	.01	.02	-.28	-.15			
13 1	.05	.16	.05	.07	.07	-.05	.11	.30	-.12			
14 1	.04	.07	-.09	.22	-.28	-.06	.23	-.31	-.06			
15 1	-.32	.13	-.27	-.24	.10	-.34	-.03	.28	-.22			
7				8				9				
?A				?A				?A				
Frequencies --	785.5269						894.5625			902.7649		
Red. masses --	1.4511						2.7967			3.8813		
Frc consts --	.5276						1.3186			1.8637		
IR Inten --	7.0357						7.5039			.5754		
Raman Activ --	.0000						.0000			.0000		
Depolar --	.0000						.0000			.0000		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z	X	Y	Z
1 7	.00	-.05	.10	.00	.16	-.09	.00	.10	-.02			
2 6	.00	-.05	-.05	.00	-.19	-.14	.00	.24	-.01			
3 6	.04	.01	.01	-.13	.07	.03	-.19	-.11	.11			
4 6	.08	.03	.01	-.05	-.07	.06	.16	-.07	-.08			
5 6	-.08	.03	.01	.05	-.07	.06	-.16	-.07	-.08			
6 6	-.04	.01	.01	.13	.07	.03	.19	-.11	.11			
7 1	.00	-.02	-.07	.00	-.28	-.09	.00	.52	-.18			
8 1	-.03	.31	-.13	-.36	.29	.23	-.23	.00	.08			
9 1	-.07	-.25	-.10	-.09	.08	.04	-.18	-.11	.10			
10 1	-.11	.35	-.14	-.18	.02	.03	.21	.03	-.14			
11 1	.10	-.24	-.25	-.10	-.23	.00	.16	-.08	-.08			
12 1	-.10	-.24	-.25	.10	-.23	.00	-.16	-.08	-.08			
13 1	.11	.35	-.14	.18	.02	.03	-.21	.03	-.14			

S25

14 1 .07 -.25 -.10 .08 .08 .04 .18 -.11 .10
 15 1 .03 .31 -.13 .36 .29 .23 .23 .00 .08

10 11 12
 ?A ?A ?A

Frequencies -- 940.3700 953.0024 989.3563

Red. masses -- 1.4385 3.4241 2.3959

Frc consts -- .7495 1.8322 1.3817

IR Inten -- .9581 13.5742 2.3432

Raman Activ -- .0000 .0000 .0000

Depolar -- .0000 .0000 .0000

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	7	-.03	.00	.00	.00	.22	.16	.06	.00	.00
2	6	.06	.00	.00	.00	-.14	.10	.02	.00	.00
3	6	.00	.02	.09	.06	.05	-.05	.01	.17	-.03
4	6	.01	-.06	-.08	.16	-.09	-.10	-.02	-.17	.06
5	6	.01	.06	.08	-.16	-.09	-.10	-.02	.17	-.06
6	6	.00	-.02	-.09	-.06	.05	-.05	.01	-.17	.03
7	1	-.23	.00	.00	.00	-.28	.19	.00	.00	.00
8	1	.20	-.01	-.21	.14	-.11	-.04	-.12	.29	.08
9	1	-.45	.16	.17	-.03	.33	.07	-.01	.28	.01
10	1	.20	-.20	-.03	-.04	-.32	.06	-.29	-.21	.12
11	1	-.05	.09	.14	.25	.04	-.12	-.02	-.32	-.06
12	1	-.05	-.09	-.14	-.25	.04	-.12	-.02	.32	.06
13	1	.20	.20	.03	.04	-.32	.06	-.29	.21	-.12
14	1	-.45	-.16	-.17	.03	.33	.07	-.01	-.28	-.01
15	1	.20	.01	.21	-.14	-.11	-.04	-.12	-.29	-.08

13 14 15
 ?A ?A ?A

Frequencies -- 1035.4994 1058.3224 1106.7663

Red. masses -- 3.3309 1.6805 1.8595

Frc consts -- 2.1043 1.1090 1.3420

IR Inten -- 2.7024 15.3502 1.0879

Raman Activ -- .0000 .0000 .0000

Depolar -- .0000 .0000 .0000

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	7	.00	.17	-.01	.16	.00	.00	.04	.00	.00
2	6	.00	-.18	.01	-.10	.00	.00	.19	.00	.00
3	6	-.05	-.18	.00	.04	-.02	.00	-.08	-.04	.06
4	6	.01	.19	.00	-.06	.03	.06	-.03	.04	.08
5	6	.00	.19	.00	-.06	-.03	-.06	-.03	-.04	-.08
6	6	.05	-.18	.00	.04	.02	.00	-.08	.04	-.06
7	1	.00	-.29	.08	-.53	.00	.00	.56	.00	.00
8	1	-.04	-.31	.07	.26	-.22	-.19	-.07	-.09	.06
9	1	.13	-.28	-.04	-.08	-.02	.01	-.26	.17	.17
10	1	.04	.24	-.02	-.27	-.14	.19	-.25	.04	.12
11	1	.08	.29	-.04	.10	.12	-.11	.19	.12	-.19
12	1	-.08	.29	-.04	.10	-.12	.11	.19	-.12	.19
13	1	-.04	.24	-.02	-.27	.14	-.19	-.25	-.04	-.12
14	1	-.13	-.28	-.04	-.08	.02	-.01	-.26	-.17	-.17
15	1	.04	-.31	.07	.26	.22	.19	-.07	.09	-.06

16 17 18
 ?A ?A ?A

Frequencies -- 1166.6949 1189.4400 1229.3648

Red. masses -- 1.9735 2.1601 1.3097

Frc consts -- 1.5827 1.8006 1.1663

IR Inten -- 1.9471 17.6246 .7481

Raman Activ -- .0000 .0000 .0000

Depolar -- .0000 .0000 .0000

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	7	.00	-.03	-.08	.23	.00	.00	.00	.01	.10
2	6	.00	.08	.14	.03	.00	.00	.00	.05	.00
3	6	-.06	.02	-.11	-.02	.00	.04	-.02	.02	-.01
4	6	.06	-.02	.09	-.13	.01	-.01	-.03	-.02	-.07
5	6	-.06	-.02	.09	-.13	-.01	.01	.03	-.02	-.07
6	6	.06	.02	-.11	-.02	.00	-.04	.02	.02	-.01
7	1	.00	-.21	.32	.26	.00	.00	.00	-.46	.32
8	1	-.13	-.14	.14	-.15	.20	.08	-.11	.12	.06
9	1	.40	.00	-.14	.03	-.19	-.04	.22	-.21	-.12
10	1	-.19	.12	.04	.29	-.01	-.07	.29	.03	-.14
11	1	.16	-.17	-.19	-.35	-.01	.32	-.21	-.04	.20
12	1	-.16	-.17	-.19	-.35	.01	-.32	.22	-.04	.20

S26

13	1	.19	.12	.04	.29	.01	.07	-.29	.03	-.14
14	1	-.40	.00	-.14	.03	.19	.04	-.22	-.21	-.12
15	1	.13	-.14	.14	-.15	-.20	-.08	.11	.12	.06
		19			20			21		
		?A			?A			?A		
Frequencies --		1244.7798				1250.7453			1268.8127	
Red. masses --		1.2620				1.2001			1.2649	
Frc consts --		1.1521				1.1062			1.1998	
IR Inten --		1.3738				.9324			.5451	
Raman Activ --		.0000				.0000			.0000	
Depolar --		.0000				.0000			.0000	
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z	
1	7	.00	.02	.02	.04	.00	.00	.00	.00	.02
2	6	.00	-.08	.09	.00	.00	.00	.00	.06	-.10
3	6	.00	.00	-.06	-.03	-.01	-.06	.00	-.03	-.02
4	6	.02	.01	.00	.01	-.01	.06	.00	-.02	.06
5	6	-.02	.01	.00	.01	.01	-.06	.00	-.02	.06
6	6	.00	.00	-.06	-.03	.01	.06	.00	-.03	-.02
7	1	.00	.46	-.23	-.14	.00	.00	.00	-.42	.19
8	1	-.02	-.09	.04	.09	-.29	-.02	.11	-.20	-.06
9	1	.02	.18	.02	-.09	.31	.08	-.24	.34	.15
10	1	.17	.22	-.13	.19	.34	-.16	.15	.29	-.14
11	1	-.30	-.29	.22	-.15	-.26	.09	.03	-.06	-.02
12	1	.30	-.29	.22	-.15	.26	-.09	-.03	-.06	-.02
13	1	-.17	.22	-.13	.19	-.34	.17	-.15	.29	-.14
14	1	-.02	.18	.02	-.09	-.31	-.08	.24	.34	.15
15	1	.02	-.09	.04	.09	.29	.02	-.11	-.20	-.06
		22			23			24		
		?A			?A			?A		
Frequencies --		1288.5080				1306.7824			1325.4534	
Red. masses --		1.5333				1.5070			1.3565	
Frc consts --		1.4999				1.5162			1.4041	
IR Inten --		4.0554				7.4849			.8295	
Raman Activ --		.0000				.0000			.0000	
Depolar --		.0000				.0000			.0000	
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z	
1	7	.00	.00	.00	.00	.00	.00	.00	.00	.00
2	6	-.04	.00	.00	.00	-.05	-.06	-.05	.00	.00
3	6	.09	-.10	-.05	-.08	.10	.05	.01	-.03	.00
4	6	-.03	.01	.01	.01	-.02	.01	.07	.09	-.04
5	6	-.03	-.01	-.01	-.01	-.02	.01	.07	-.09	.04
6	6	.10	.10	.06	.08	.10	.05	.01	.03	.00
7	1	-.22	.00	.00	.00	.03	-.12	.20	.00	.00
8	1	-.29	.37	.18	.37	-.44	-.21	-.01	-.01	.01
9	1	-.26	.30	.14	.15	-.23	-.10	-.11	.10	.07
10	1	.04	.04	-.02	.04	.05	-.04	-.29	-.22	.19
11	1	.06	.12	-.05	-.01	-.06	.02	-.34	-.32	.22
12	1	.06	-.12	.05	.01	-.06	.02	-.34	.32	-.22
13	1	.04	-.05	.02	-.04	.05	-.04	-.29	.22	-.19
14	1	-.26	-.30	-.14	-.15	-.23	-.10	-.11	-.11	-.07
15	1	-.29	-.37	-.18	-.37	-.44	-.21	-.01	.01	-.01
		25			26			27		
		?A			?A			?A		
Frequencies --		1351.1292				1395.5795			1535.9670	
Red. masses --		1.3902				1.5930			1.0920	
Frc consts --		1.4953				1.8280			1.5179	
IR Inten --		1.2873				4.4513			1.4531	
Raman Activ --		.0000				.0000			.0000	
Depolar --		.0000				.0000			.0000	
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z	
1	7	.00	-.04	.01	-.01	.00	.00	.01	.00	.00
2	6	.00	.04	-.05	.21	.00	.00	.01	.00	.00
3	6	-.02	-.02	.01	-.06	-.01	-.01	-.03	-.04	.02
4	6	.07	.09	-.03	.02	.03	-.01	.01	-.02	-.01
5	6	-.07	.09	-.03	.02	-.03	.01	.01	.02	.01
6	6	.02	-.02	.01	-.06	.01	.01	-.03	.04	-.02
7	1	.00	-.25	.12	-.84	.00	.00	-.02	.00	.00
8	1	.03	-.07	-.02	-.18	.02	.14	.07	.25	-.37
9	1	-.08	.05	.05	.09	-.12	-.06	.36	.25	.11
10	1	-.31	-.24	.21	-.13	-.03	.05	-.17	.13	-.05
11	1	-.30	-.34	.17	-.10	-.05	.10	-.03	.14	.16

S27

12	1	.30	-.34	.17	-.10	.05	-.10	-.03	-.14	-.16
13	1	.31	-.24	.21	-.13	.03	-.05	-.17	-.13	.05
14	1	.08	.05	.05	.09	.12	.06	.36	-.25	-.11
15	1	-.03	-.07	-.02	-.18	-.02	-.14	.07	-.25	.37
		28			29			30		
		?A			?A			?A		
Frequencies --		1546.8603			1560.3714			1579.8465		
Red. masses --		1.0929			1.1124			1.1067		
Frc consts --		1.5408			1.5958			1.6274		
IR Inten --		2.6449			.0338			4.3015		
Raman Activ --		.0000			.0000			.0000		
Depolar --		.0000			.0000			.0000		
Atom AN		X	Y	Z	X	Y	Z	X	Y	Z
1	7	.00	.00	.00	.01	.00	.00	.00	.01	.00
2	6	.00	-.01	-.01	-.02	.00	.00	.00	-.01	.00
3	6	-.04	-.04	.02	.02	.02	-.01	-.02	-.02	.01
4	6	.01	-.01	-.01	.03	-.05	-.02	-.03	.05	.02
5	6	-.01	-.01	-.01	.03	.05	.02	.03	.05	.02
6	6	.04	-.04	.02	.02	-.02	.01	.02	-.02	.01
7	1	.00	.00	-.01	.06	.00	.00	.00	.01	-.02
8	1	.09	.25	-.38	-.02	-.12	.16	.04	.09	-.16
9	1	.37	.24	.11	-.17	-.11	-.05	.15	.10	.05
10	1	-.16	.10	-.04	-.35	.27	-.11	.38	-.25	.10
11	1	-.02	.13	.14	-.03	.30	.34	.04	-.29	-.35
12	1	.02	.13	.14	-.03	-.30	-.34	-.04	-.29	-.35
13	1	.16	.10	-.04	-.35	-.27	.11	-.38	-.25	.11
14	1	-.37	.24	.11	-.17	.11	.05	-.15	.10	.05
15	1	-.09	.25	-.38	-.02	.12	-.16	-.04	.09	-.16
		31			32			33		
		?A			?A			?A		
Frequencies --		3096.2307			3099.4092			3121.8576		
Red. masses --		1.0607			1.0604			1.0631		
Frc consts --		5.9914			6.0015			6.1047		
IR Inten --		22.2278			80.5898			31.6225		
Raman Activ --		.0000			.0000			.0000		
Depolar --		.0000			.0000			.0000		
Atom AN		X	Y	Z	X	Y	Z	X	Y	Z
1	7	.00	.00	.00	.00	.00	.00	.00	.00	.00
2	6	.00	.00	.00	.00	.00	-.01	.00	.02	.03
3	6	.00	.00	.00	.00	.00	.01	-.03	-.03	.02
4	6	.01	-.04	-.03	.02	-.04	-.03	.00	.00	.00
5	6	.01	.04	.03	-.02	-.04	-.03	.00	.00	.00
6	6	.00	.00	.00	.00	.00	.01	.02	-.03	.02
7	1	.00	.00	.00	.00	.04	.07	.00	-.21	-.35
8	1	.02	.01	.01	.03	.02	.02	.33	.16	.22
9	1	.00	.02	-.06	-.01	.03	-.08	-.03	.19	-.46
10	1	.10	.28	.53	.09	.27	.51	-.01	-.02	-.04
11	1	-.27	.14	-.19	-.27	.14	-.19	.03	-.02	.02
12	1	-.26	-.14	.19	.28	.15	-.19	-.03	-.01	.02
13	1	.10	-.28	-.52	-.09	.28	.53	.01	-.02	-.04
14	1	.00	-.02	.05	.01	.03	-.08	.03	.18	-.44
15	1	.02	-.01	-.01	-.03	.02	.02	-.32	.16	.21
		34			35			36		
		?A			?A			?A		
Frequencies --		3123.1844			3132.5118			3160.1545		
Red. masses --		1.0614			1.0877			1.1082		
Frc consts --		6.1001			6.2882			6.5207		
IR Inten --		22.9171			32.4469			19.9344		
Raman Activ --		.0000			.0000			.0000		
Depolar --		.0000			.0000			.0000		
Atom AN		X	Y	Z	X	Y	Z	X	Y	Z
1	7	.00	.00	.00	.00	.00	.00	.00	.00	.00
2	6	.00	.00	.00	.00	-.04	-.07	.00	.00	.00
3	6	.02	.03	-.03	-.01	-.01	.02	.01	.00	.02
4	6	.00	.00	.00	.00	.01	.00	-.04	.01	-.05
5	6	.00	.00	.00	.00	.01	.00	-.04	-.01	.05
6	6	.02	-.03	.03	.01	-.01	.02	.01	.00	-.02
7	1	.00	.00	-.01	.00	.47	.76	.00	.00	.00
8	1	-.31	-.15	-.21	.08	.04	.05	-.13	-.07	-.08
9	1	.04	-.22	.51	-.02	.11	-.26	.00	.04	-.10
10	1	.01	.02	.04	-.01	-.03	-.06	.05	.16	.29

S28

11	1	-.03	.02	-.02	.04	-.02	.03	.45	-.25	.30
12	1	-.03	-.02	.02	-.04	-.02	.03	.44	.25	-.29
13	1	.01	-.02	-.04	.01	-.03	-.06	.04	-.16	-.28
14	1	.04	.22	-.53	.02	.11	-.26	.00	-.04	.10
15	1	-.32	.16	.22	-.08	.04	.05	-.13	.06	.08

		37				38			39	
		?A				?A			?A	

Frequencies --	3162.4645		3189.1797		3193.1723
Red. masses --	1.1084		1.1084		1.1081
Frc consts --	6.5313		6.6419		6.6568
IR Inten --	12.7029		24.9280		38.5621
Raman Activ --	.0000		.0000		.0000
Depolar --	.0000		.0000		.0000

Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 7	.00	.00	.00	.00	.00	.00	.00	.00	.00
2 6	.00	.00	.00	.00	.00	.00	.00	.01	.01
3 6	.01	.00	.02	.04	.01	.05	.04	.00	.05
4 6	-.04	.01	-.05	.01	.00	.02	.01	.00	.02
5 6	.04	.01	-.05	.01	.00	-.01	-.01	.00	.02
6 6	-.01	.00	.02	.04	-.01	-.05	-.04	.00	.05
7 1	.00	-.03	-.04	.00	.00	.00	.00	-.07	-.11
8 1	-.14	-.07	-.09	-.43	-.22	-.27	-.41	-.21	-.26
9 1	.00	.05	-.11	-.02	.16	-.36	-.01	.16	-.36
10 1	.04	.16	.29	-.02	-.06	-.10	-.02	-.06	-.10
11 1	.43	-.24	.29	-.13	.07	-.08	-.13	.08	-.09
12 1	-.44	-.25	.29	-.12	-.07	.08	.14	.08	-.09
13 1	-.04	.17	.30	-.02	.06	.10	.02	-.06	-.11
14 1	.00	.05	-.11	-.02	-.16	.36	.02	.16	-.37
15 1	.14	-.07	-.09	-.42	.22	.26	.42	-.21	-.26

- Thermochemistry -

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Atom 1 has atomic number 7 and mass 14.00307

Atom 2 has atomic number 6 and mass 12.00000

Atom 3 has atomic number 6 and mass 12.00000

Atom 4 has atomic number 6 and mass 12.00000

Atom 5 has atomic number 6 and mass 12.00000

Atom 6 has atomic number 6 and mass 12.00000

Atom 7 has atomic number 1 and mass 1.00783

Atom 8 has atomic number 1 and mass 1.00783

Atom 9 has atomic number 1 and mass 1.00783

Atom 10 has atomic number 1 and mass 1.00783

Atom 11 has atomic number 1 and mass 1.00783

Atom 12 has atomic number 1 and mass 1.00783

Atom 13 has atomic number 1 and mass 1.00783

Atom 14 has atomic number 1 and mass 1.00783

Atom 15 has atomic number 1 and mass 1.00783

Molecular mass: 83.07350 amu.

Principal axes and moments of inertia in atomic units:

	1	2	3
EIGENVALUES --	278.78220	436.44740	570.36482
X	1.00000	.00000	.00000
Y	.00000	.99906	.04342
Z	.00000	-.04342	.99906

THIS MOLECULE IS AN ASYMMETRIC TOP.

ROTATIONAL SYMMETRY NUMBER 1.

ROTATIONAL TEMPERATURES (KELVIN) .31068 .19845 .15186

ROTATIONAL CONSTANTS (GHZ) 6.47366 4.13507 3.16419

1 IMAGINARY FREQUENCIES IGNORED.

Zero-point vibrational energy 359676.1 (Joules/Mol)

85.96464 (Kcal/Mol)

WARNING-- EXPLICIT CONSIDERATION OF 2 DEGREES OF FREEDOM AS
VIBRATIONS MAY CAUSE SIGNIFICANT ERRORVIBRATIONAL TEMPERATURES: 464.05 607.47 987.41 1059.34 1123.88
(KELVIN) 1130.19 1287.07 1298.87 1352.97 1371.15

1423.45 1489.84 1522.68 1592.38 1678.60

1711.33 1768.77 1790.95 1799.53 1825.53

1853.86 1880.16 1907.02 1943.96 2007.92

2209.90 2225.57 2245.01 2273.03 4454.76

4459.33 4491.63 4493.54 4506.96 4546.73
4550.05 4588.49 4594.24

Zero-point correction= .136993 (Hartree/Particle)
Thermal correction to Energy= .141371
Thermal correction to Enthalpy= .142315
Thermal correction to Gibbs Free Energy= .109374
Sum of electronic and zero-point Energies= -249.615045
Sum of electronic and thermal Energies= -249.610668
Sum of electronic and thermal Enthalpies= -249.609724
Sum of electronic and thermal Free Energies= -249.642665

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	88.712	17.248	69.331
ELECTRONIC	.000	.000	.000
TRANSLATIONAL	.889	2.981	39.165
ROTATIONAL	.889	2.981	25.743
VIBRATIONAL	86.934	11.286	4.423
VIBRATION 1	.708	1.630	1.297
VIBRATION 2	.785	1.422	.884
	Q	LOG10(Q)	LN(Q)
TOTAL BOT	.491897D-50	-50.308126	-115.838740
TOTAL V=0	.505854D+13	12.704025	29.252099
VIB (BOT)	.175265D-62	-62.756304	-144.501730
VIB (BOT) 1	.581952D+00	-.235113	-.541368
VIB (BOT) 2	.415173D+00	-.381771	-.879061
VIB (V=0)	.180238D+01	.255847	.589109
VIB (V=0) 1	.126725D+01	.102861	.236847
VIB (V=0) 2	.114990D+01	.060660	.139674
ELECTRONIC	.100000D+01	.000000	.000000
TRANSLATIONAL	.297615D+08	7.473654	17.208725
ROTATIONAL	.943027D+05	4.974524	11.454265

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr)		
		X	Y	Z
1	7	.000008130	-.000009556	.000000898
2	6	.000007401	-.000012921	-.000005684
3	6	.000004864	.000012660	.0000006170
4	6	-.000005931	.000007985	-.000009589
5	6	-.000009139	.000013109	-.000009095
6	6	.000001941	-.000000553	.0000006317
7	1	-.000000758	-.000000563	.000002090
8	1	-.000010223	-.000012264	-.000001886
9	1	-.000006117	.000002595	-.000001150
10	1	-.000000777	.000000668	.000004557
11	1	.000000850	-.000005458	.000003899
12	1	.000001991	-.000002998	.000002844
13	1	.000001183	-.000000834	.000000801
14	1	-.000000493	.000003674	-.000001492
15	1	.000007078	.000004456	.000001320

Cartesian Forces: Max .000013109 RMS .000006138
1\1\GINC-ARMON\Freq\RMP2-FC\6-31G(d)\C5H9N1\BELOSTOT\20-Sep-2002\0\#\n
MP2/6-31G* OPT=(NEWTON, CARTESIAN, TS, CALCALL) GUESS=CHECKPOINT GEOM=
ALLCHECKPOINT\1-azabicyclo220hexane, RI TS\0,1\N,-0.3259902826,0.519
7085993,-0.7772487902\C,-0.3020276069,0.481053507,0.7452038886\C,1.235
7425523,0.5010997968,0.7672665956\C,1.1726252697,0.4619755609,-0.77701
04728\C,-0.9262284369,-0.8546448107,-0.7774596324\C,-0.9883444612,-0.8
952482857,0.7668196195\H,-0.8122629786,1.2935228607,1.2741981863\H,1.6
636327223,1.4208226219,1.1742644903\H,1.7109397026,-0.3525253762,1.261
1102205\H,1.5747592551,-0.4432003915,-1.2483734343\H,1.6085493828,1.33
21376203,-1.2770671073\H,-1.8996276328,-0.8680283624,-1.2770371479\H,-
0.2865905521,-1.6104133198,-1.2495752399\H,-0.4256554188,-1.6943407833
,1.2599741988\H,-2.0024164039,-0.8813496742,1.1743273738\Version=IBM-
RS6000-G98RevA.7\HF=-248.9419519\MP2=-249.7520387\RMSE=1.173e-09\RMSE=
6.138e-06\Dipole=0.2792023,-0.4452246,0.4300424\

Pyrrolizidine 4 (cis-conformer)CONFORMATIONAL ENERGY, PART 3: GEOMETRY AND STERIC ENERGY
OF FINAL CONFORMATION.

CONNECTED ATOMS

1- 2- 3- 4- 5- 1-
2- 6- 8- 7-
3- 7-

ATTACHED ATOMS

1- 9, 1- 10, 2- 11, 4- 12, 4- 13, 5- 14, 5- 15,
6- 16, 6- 17, 7- 18, 7- 19, 8- 20, 8- 21,

FINAL ATOMIC COORDINATE

ATOM	X	Y	Z	TYPE
C(1)	-.90683	1.25960	.45808	(1)
C(2)	.10173	.79027	-.61072	(1)
N(3)	-.06504	-.66581	-.60314	(8)
C(4)	-1.48996	-.95679	-.42798	(1)
C(5)	-2.01640	.17744	.47786	(1)
C(6)	1.58753	.98858	-.24274	(1)
C(7)	.76956	-1.20161	.47514	(1)
C(8)	2.05073	-.35931	.37005	(1)
H(9)	-.42393	1.32513	1.45896	(5)
H(10)	-1.31436	2.26562	.21428	(5)
H(11)	-.15278	1.20164	-1.61297	(5)
H(12)	-1.99489	-.91313	-1.41913	(5)
H(13)	-1.65891	-1.97084	-.00266	(5)
H(14)	-2.18866	-.18731	1.51556	(5)
H(15)	-2.98034	.57805	.09164	(5)
H(16)	2.18673	1.22033	-1.15227	(5)
H(17)	1.71676	1.83210	.47049	(5)
H(18)	.28637	-1.04909	1.47833	(5)
H(19)	.96171	-2.28741	.33456	(5)
H(20)	2.53632	-.22302	1.36163	(5)
H(21)	2.78244	-.85453	-.30836	(5)

THIS MOLECULE CONTAINS

2 5-MEMBERED RING(S)

DIELECTRIC CONSTANT = 1.500

BOND LENGTHS AND STRETCHING ENERGY (22 BONDS)

ENERGY = 71.94(KS)(DR)(DR)(1-(CS)(DR)+(7/12)((CS)(DR))**2)
DR = R-RO
CS = 2.550

BOND	LENGTH	R(0)	R(0)-CORR K(S)	CORR ENERGY	E-NEG	MISCEL	KS
C(1)- C(2)	1.5427	1.5208	4.490	.1460	-.0050		
C(1)- C(5)	1.5500	1.5226	4.490	.2274	-.0032		
C(1)- H(9)	1.1132	1.1116	4.694	.0009	-.0004	.014	
C(1)- H(10)	1.1125	1.1116	4.694	.0003	-.0004	.014	
C(2)- N(3)	1.4656	1.4530	5.300	.0588			
C(2)- C(6)	1.5435	1.5208	4.490	.1569	-.0050		
C(2)- H(11)	1.1129	1.1114	4.831	.0008	-.0011	.0005 BH	.021
N(3)- C(4)	1.4648	1.4530	5.300	.0518			
N(3)- C(7)	1.4650	1.4530	5.300	.0536			
C(4)- C(5)	1.5441	1.5208	4.490	.1650	-.0050		
C(4)- H(12)	1.1132	1.1114	4.701	.0012	-.0011	.0005 BH	.021
C(4)- H(13)	1.1125	1.1124	4.666	.0000	-.0011	.0015 BH	.014
C(5)- H(14)	1.1133	1.1116	4.694	.0011	-.0004	.014	
C(5)- H(15)	1.1130	1.1116	4.694	.0007	-.0004	.014	
C(6)- C(8)	1.5514	1.5226	4.490	.2500	-.0032		
C(6)- H(16)	1.1136	1.1116	4.694	.0013	-.0004	.014	
C(6)- H(17)	1.1122	1.1116	4.694	.0001	-.0004	.014	
C(7)- C(8)	1.5368	1.5208	4.490	.0799	-.0050		

S31

C(7)- H(18) 1.1239 1.1225 4.337 .0006 -.0011 .0116 BH -.343
 C(7)- H(19) 1.1116 1.1113 4.702 .0000 -.0011 .0004 BH .022
 C(8)- H(20) 1.1125 1.1116 4.694 .0003 -.0004 .014
 C(8)- H(21) 1.1139 1.1116 4.694 .0019 -.0004 .014

NON-BONDED DISTANCES, VDW AND EPR ENERGY (143 PAIRS)

$E(\text{VDW}) = KV \cdot (1.84(10^{**5}) \cdot \exp(-12.00/P) - 2.25(P^{**6}))$
 $E(\text{EPR}) = C \cdot KV \cdot (1.84(10^{**5}) \cdot \exp(-12.00/Q) - 2.25(Q^{**6}))$
 $E(\text{HBD}) = EP1 - EP2 \cdot \cos(\text{THETA}) \cdot RTH/RTH0$
 $EP1 = KHB \cdot 1.84(10^{**5}) \cdot \exp(-12.0/P)$
 $EP2 = KHB \cdot 2.25(P^{**6})$

IF P > 3.020, THEN,

$E(\text{VDW}) = KV(192.270)(P^{**2})$
 $E(\text{HBD}) = EP1 - EP2 \cdot \cos(\text{THETA}) \cdot RTH/RTH0$
 $EP1 = KHB \cdot (192.270 \cdot P^{**2} + 1706.96)$
 $EP2 = KHB \cdot 1706.96$

WHERE RV = RVDW(I) + RVDW(K)

KV = SQRT(EPS(I) * EPS(K))

KHB = EPS/DIELEC FOR HYDROGEN BOND

P = (RV/R) OR (RV/R#)

C = SCALE FACTOR

Q = RV/R, WHERE R IS MODIFIED DISTANCE

THETA = ANGLE H-X-Y IN HYDROGEN BOND X-H...Y

RTH = BOND LENGTH X-H IN X-H...Y

RTH0 = NATURAL BOND LENGTH X-H

IN THE VDW CALCULATIONS THE HYDROGEN ATOMS ARE RELOCATED
 SO THAT THE ATTACHED HYDROGEN DISTANCE IS REDUCED BY .923

IN THE VDW CALCULATIONS THE DEUTERIUM ATOMS ARE RELOCATED
 SO THAT THE ATTACHED DEUTERIUM DISTANCE IS REDUCED BY .923

** INTERACTIONS OF LESS THAN 0.1 KCAL/MOL ARE NOT PRINTED **

ATOM PAIR	R	R#	RV	KV	ENERGY
C(1), C(7)	2.9779		4.080	.0270	.3787 1,4
C(1), H(17)	2.6854	2.6628	3.560	.0230	.2396 1,4
C(1), H(18)	2.7919	2.7906	3.560	.0230	.1247
C(2), H(12)	2.8197	2.7719	3.560	.0230	.1382 1,4
C(2), H(18)	2.7895	2.7428	3.560	.0230	.1612 1,4
N(3), H(9)	2.8888	2.8357	3.550	.0293	.1168 1,4
N(3), H(21)	2.8689	2.8167	3.550	.0293	.1310 1,4
C(4), H(11)	2.8020	2.7552	3.560	.0230	.1511 1,4
C(4), H(18)	2.6073	2.5778	3.560	.0230	.3536 1,4
C(5), C(7)	3.1086		4.080	.0270	.2209 1,4
C(5), H(18)	2.7943	2.8038	3.560	.0230	.1159
C(6), H(9)	2.6561	2.6356	3.560	.0230	.2722 1,4
C(7), H(13)	2.5918	2.5637	3.560	.0230	.3762 1,4
H(9), H(14)	2.3249	2.2650	3.240	.0200	.4513 1,4
H(9), H(17)	2.4118	2.4153	3.240	.0200	.2174
H(9), H(18)	2.4783	2.5070	3.240	.0200	.1318
H(10), H(11)	2.4125	2.3426	3.240	.0200	.3128 1,4
H(10), H(15)	2.3745	2.3108	3.240	.0200	.3643 1,4
H(11), H(16)	2.3845	2.3188	3.240	.0200	.3507 1,4
H(12), H(15)	2.3403	2.2779	3.240	.0200	.4250 1,4
H(13), H(14)	2.4014	2.3344	3.240	.0200	.3254 1,4
H(16), H(21)	2.3178	2.2586	3.240	.0200	.4647 1,4
H(17), H(20)	2.3852	2.3209	3.240	.0200	.3472 1,4
H(18), H(20)	2.3996	2.3302	3.240	.0200	.3320 1,4
H(19), H(21)	2.4045	2.3350	3.240	.0200	.3245 1,4

BOND ANGLES, BENDING AND STRETCH-BEND ENERGIES (45 ANGLES)

$EB = 0.021914(KB)(DT)(DT)(1 + CF \cdot DT + QF \cdot DT^{**2} + PF \cdot DT^{**3} + SF \cdot DT^{**4})$
 DT = THETA-TZERO
 CF = -1400.000E-5

QF = 5.600E-5
 PF = -.070E-5
 SF = .022E-6
 ESB(J) = 2.51124(KSB(J))(DT)(DR1+DR2)
 DR(I) = R(I) - R0(I)
 EBDDBD = -0.02191418(KBB1)(DT1)(KBB2)(DT2)

A T O M S			THETA	TZERO	KB	EB	KSB	ESB
C(2)-C(1)-C(5)	105.334	111.000	.670	.5097	.13	-.0912		
C(2)-C(1)-H(9)	110.930	109.310	.590	.0332	.08	.0076		
C(2)-C(1)-H(10)	111.271	109.310	.590	.0484	.08	.0090		
C(5)-C(1)-H(9)	109.886	109.310	.590	.0043	.08	.0034		
C(5)-C(1)-H(10)	111.833	109.310	.590	.0794	.08	.0144		
H(9)-C(1)-H(10)	107.621	107.600	.550	.0000				
C(1)-C(2)-N(3)	102.960	108.000	.780	.4654	.13	-.0567		
C(1)-C(2)-C(6)	115.156	110.200	.670	.3361	.13	.0721		
C(1)-C(2)-H(11)	111.222	109.800	.590	.0256	.08	.0067		
N(3)-C(2)-C(6)	103.647	108.000	.780	.3440	.13	-.0502		
N(3)-C(2)-H(11)	110.235	109.300	.820	.0155	.08	.0027		
C(6)-C(2)-H(11)	112.791	109.800	.590	.1108	.08	.0145		
C(2)-N(3)-C(4)	107.978	114.000	.720	.6217	.10	-.0370		
C(2)-N(3)-C(7)	107.598	114.000	.720	.7063	.10	-.0396		
C(4)-N(3)-C(7)	113.172	107.200	.720	.5167	.05	.0179		
N(3)-C(4)-C(5)	104.826	109.700	.780	.4343	.13	-.0559		
N(3)-C(4)-H(12)	109.085	109.300	.820	.0008	.08	-.0006		
N(3)-C(4)-H(13)	111.993	109.300	.820	.1255	.08	.0065		
C(5)-C(4)-H(12)	109.808	109.310	.590	.0032	.08	.0025		
C(5)-C(4)-H(13)	113.172	109.310	.590	.1826	.08	.0181		
H(12)-C(4)-H(13)	107.893	107.600	.550	.0010				
C(1)-C(5)-C(4)	105.147	111.000	.670	.5453	.13	-.0970		
C(1)-C(5)-H(14)	110.572	109.310	.590	.0202	.08	.0074		
C(1)-C(5)-H(15)	111.361	109.310	.590	.0528	.08	.0119		
C(4)-C(5)-H(14)	111.032	109.310	.590	.0374	.08	.0087		
C(4)-C(5)-H(15)	110.861	109.310	.590	.0304	.08	.0077		
H(14)-C(5)-H(15)	107.900	107.600	.550	.0011				
C(2)-C(6)-C(8)	105.661	111.000	.670	.4505	.13	-.0898		
C(2)-C(6)-H(16)	110.488	109.310	.590	.0176	.08	.0058		
C(2)-C(6)-H(17)	111.235	109.310	.590	.0466	.08	.0090		
C(8)-C(6)-H(16)	110.046	109.310	.590	.0069	.08	.0046		
C(8)-C(6)-H(17)	111.774	109.310	.590	.0758	.08	.0146		
H(16)-C(6)-H(17)	107.664	107.600	.550	.0000				
N(3)-C(7)-C(8)	102.952	109.700	.780	.8541	.13	-.0619		
N(3)-C(7)-H(18)	111.249	109.300	.820	.0664	.08	.0053		
N(3)-C(7)-H(19)	111.262	109.300	.820	.0673	.08	.0049		
C(8)-C(7)-H(18)	110.185	109.310	.590	.0098	.08	.0031		
C(8)-C(7)-H(19)	112.495	109.310	.590	.1254	.08	.0104		
H(18)-C(7)-H(19)	108.649	107.600	.550	.0131				
C(6)-C(8)-C(7)	104.731	111.000	.670	.6290	.13	-.0919		
C(6)-C(8)-H(20)	112.082	109.310	.590	.0956	.08	.0166		
C(6)-C(8)-H(21)	109.987	109.310	.590	.0059	.08	.0042		
C(7)-C(8)-H(20)	111.720	109.310	.590	.0726	.08	.0082		
C(7)-C(8)-H(21)	110.217	109.310	.590	.0105	.08	.0034		
H(20)-C(8)-H(21)	108.094	107.600	.550	.0029				

DIHEDRAL ANGLES, TORSIONAL ENERGY (ET) (72 ANGLES)

$$ET = (V1/2)(1+\cos(W)) + (V2/2)(1-\cos(2W)) + (V3/2)(1+\cos(3W))$$

$$ETS = -11.995*(R-R0)((KTS1/2)(1+\cos(W)) + (KTS2/2)(1-\cos(2W)) + (KTS3/2)(1+\cos(3W)))$$

SIGN OF ANGLE A-B-C-D : WHEN LOOKING THROUGH B TOWARD C,
IF D IS COUNTERCLOCKWISE FROM A, NEGATIVE.

A T O M S			OMEGA	V1	V2	V3	ET	KTS3	ETS
C(1)C(2)N(3)C(4)	38.3	.958	-.155	1.360	1.190	.061	-.003		
C(1)C(2)N(3)C(7)	-84.2	.958	-.155	.766	.642	.061	-.003		
C(1)C(2)C(6)C(8)	94.7	.185	.170	.520	.577	.059	-.010		
C(1)C(2)C(6)H(16)	-146.3	.000	.000	.280	.167	.059	-.010		

C(1) C(2) C(6) H(17) -26.8 .000 .000 .280 .163 .059 -.009
C(1) C(5) C(4) N(3) 14.5 -.302 .696 1.360 .920 .059 -.014
C(1) C(5) C(4) H(12) -102.6 .000 .000 .280 .226 .059 -.013
C(1) C(5) C(4) H(13) 136.8 .000 .000 .280 .229 .059 -.013
C(2) C(1) C(5) C(4) 8.0 .185 .170 1.160 1.298 .059 -.019
C(2) C(1) C(5) H(14) 127.9 .000 .000 .280 .268 .059 -.019
C(2) C(1) C(5) H(15) -112.2 .000 .000 .280 .268 .059 -.019
C(2) N(3) C(4) C(5) -33.5 .958 -.155 1.360 1.388 .061 -.004
C(2) N(3) C(4) H(12) 84.1 .072 -.012 .563 .223 .061 -.003
C(2) N(3) C(4) H(13) -156.6 .072 -.012 .563 .188 .061 -.003
C(2) N(3) C(7) C(8) -40.4 .958 -.155 1.360 1.107 .061 -.002
C(2) N(3) C(7) H(18) 77.6 .072 -.012 .563 .144 .061 -.002
C(2) N(3) C(7) H(19) -161.1 .072 -.012 .563 .128 .061 -.002
C(2) C(6) C(8) C(7) -6.5 .185 .170 1.160 1.313 .059 -.020
C(2) C(6) C(8) H(20) -127.8 .000 .000 .280 .268 .059 -.020
C(2) C(6) C(8) H(21) 111.9 .000 .000 .280 .268 .059 -.020
N(3) C(2) C(1) C(5) -27.4 -.302 .696 1.360 .635 .059 -.009
N(3) C(2) C(1) H(9) 91.5 .000 .000 .374 .201 .059 -.008
N(3) C(2) C(1) H(10) -148.8 .000 .000 .374 .199 .059 -.008
N(3) C(2) C(6) C(8) -17.0 -.302 .696 1.360 .873 .059 -.013
N(3) C(2) C(6) H(16) 102.0 .000 .000 .374 .297 .059 -.013
N(3) C(2) C(6) H(17) -138.5 .000 .000 .374 .293 .059 -.013
N(3) C(4) C(5) H(14) -105.1 .000 .000 .374 .320 .059 -.014
N(3) C(4) C(5) H(15) 135.0 .000 .000 .374 .319 .059 -.014
N(3) C(7) C(8) C(6) 27.6 -.302 .696 1.360 .631 .059 -.006
N(3) C(7) C(8) H(20) 149.1 .000 .000 .374 .196 .059 -.006
N(3) C(7) C(8) H(21) -90.7 .000 .000 .374 .194 .059 -.006
C(4) N(3) C(2) C(6) 158.6 .958 -.155 .766 .229 .061 -.003
C(4) N(3) C(2) H(11) -80.4 .072 -.012 .563 .177 .061 -.002
C(4) N(3) C(7) C(8) -159.6 .958 -.155 .766 .210 .061 -.002
C(4) N(3) C(7) H(18) -41.6 .072 -.012 .563 .178 .061 -.002
C(4) N(3) C(7) H(19) 79.7 .072 -.012 .563 .168 .061 -.002
C(4) C(5) C(1) H(9) -111.6 .000 .000 .280 .267 .059 -.019
C(4) C(5) C(1) H(10) 129.0 .000 .000 .280 .265 .059 -.018
C(5) C(1) C(2) C(6) -139.5 .185 .170 .520 .490 .059 -.012
C(5) C(1) C(2) H(11) 90.6 .000 .000 .280 .145 .059 -.008
C(5) C(4) N(3) C(7) 85.5 .958 -.155 .766 .656 .061 -.003
C(6) C(2) C(1) H(9) -20.6 .000 .000 .280 .206 .059 -.011
C(6) C(2) C(1) H(10) 99.2 .000 .000 .280 .205 .059 -.011
C(6) C(2) N(3) C(7) 36.1 .958 -.155 1.360 1.278 .061 -.003
C(6) C(8) C(7) H(18) -91.2 .000 .000 .280 .149 .059 -.006
C(6) C(8) C(7) H(19) 147.4 .000 .000 .280 .159 .059 -.006
C(7) N(3) C(2) H(11) 157.1 .072 -.012 .563 .181 .061 -.003
C(7) N(3) C(4) H(12) -156.9 .072 -.012 .563 .182 .061 -.003
C(7) N(3) C(4) H(13) -37.6 .072 -.012 .563 .233 .061 -.003
C(7) C(8) C(6) H(16) -125.8 .000 .000 .280 .274 .059 -.020
C(7) C(8) C(6) H(17) 114.6 .000 .000 .280 .275 .059 -.020
C(8) C(6) C(2) H(11) -136.2 .000 .000 .280 .233 .059 -.013
H(9) C(1) C(2) H(11) -150.5 .000 .000 .238 .116 .059 -.008
H(9) C(1) C(5) H(14) 8.3 .000 .000 .238 .227 .059 -.019
H(9) C(1) C(5) H(15) 128.3 .000 .000 .238 .227 .059 -.019
H(10) C(1) C(2) H(11) -30.7 .000 .000 .238 .114 .059 -.007
H(10) C(1) C(5) H(14) -111.1 .000 .000 .238 .225 .059 -.018
H(10) C(1) C(5) H(15) 8.8 .000 .000 .238 .226 .059 -.018
H(11) C(2) C(6) H(16) -17.2 .000 .000 .238 .193 .059 -.013
H(11) C(2) C(6) H(17) 102.3 .000 .000 .238 .191 .059 -.013
H(12) C(4) C(5) H(14) 137.8 .000 .000 .238 .190 .059 -.013
H(12) C(4) C(5) H(15) 17.9 .000 .000 .238 .189 .059 -.013
H(13) C(4) C(5) H(14) 17.2 .000 .000 .238 .193 .059 -.013
H(13) C(4) C(5) H(15) -102.7 .000 .000 .238 .193 .059 -.013
H(16) C(6) C(8) H(20) 112.9 .000 .000 .238 .230 .059 -.020
H(16) C(6) C(8) H(21) -7.4 .000 .000 .238 .229 .059 -.020
H(17) C(6) C(8) H(20) -6.7 .000 .000 .238 .231 .059 -.020
H(17) C(6) C(8) H(21) -127.0 .000 .000 .238 .230 .059 -.020
H(18) C(7) C(8) H(20) 30.4 .000 .000 .238 .117 .059 -.006
H(18) C(7) C(8) H(21) 150.6 .000 .000 .238 .115 .059 -.006
H(19) C(7) C(8) H(20) -91.0 .000 .000 .238 .125 .059 -.006
H(19) C(7) C(8) H(21) 29.2 .000 .000 .238 .124 .059 -.006

=====

NORMAL MODE VIBRATIONAL ANALYSIS

Molecular Shape : ASYMMETRIC ROTOR WITH KAPPA = -.626937
 Symmetry Point Group : C1
 Symmetry Number : 1
 Chirality : yes

0 FUNDAMENTAL NORMAL VIBRATIONAL FREQUENCIES
(THEORETICALLY 57 VALUES)

Frequency : in 1/cm
 A(i) : IR intensity (vs,s,m,w,vw,-- or in 10**6 cm/mole)
 A(i) = -- : IR inactive

no	Frequency	Symmetry	A(i)
1.	2958.6	(A)	m
2.	2947.7	(A)	s
3.	2947.4	(A)	m
4.	2945.6	(A)	w
5.	2942.1	(A)	w
6.	2939.9	(A)	w
7.	2938.8	(A)	m
8.	2896.1	(A)	m
9.	2892.6	(A)	m
10.	2889.0	(A)	m
11.	2880.8	(A)	m
12.	2879.7	(A)	w
13.	2797.6	(A)	m
14.	1503.0	(A)	w
15.	1471.2	(A)	w
16.	1427.2	(A)	w
17.	1417.1	(A)	w
18.	1408.6	(A)	w
19.	1408.1	(A)	w
20.	1394.3	(A)	w
21.	1386.7	(A)	w
22.	1363.3	(A)	w
23.	1357.1	(A)	w
24.	1322.4	(A)	w
25.	1317.6	(A)	w
26.	1303.2	(A)	w
27.	1281.9	(A)	w
28.	1268.4	(A)	w
29.	1246.9	(A)	w
30.	1186.9	(A)	w
31.	1171.3	(A)	w
32.	1168.6	(A)	w
33.	1137.2	(A)	w
34.	1119.7	(A)	w
35.	1107.9	(A)	w
36.	1035.8	(A)	w
37.	1012.7	(A)	w
38.	1006.3	(A)	vw
39.	973.3	(A)	w
40.	962.3	(A)	w
41.	943.4	(A)	w
42.	899.6	(A)	w
43.	883.2	(A)	w
44.	857.9	(A)	w
45.	843.4	(A)	w
46.	798.6	(A)	w
47.	765.2	(A)	w
48.	759.7	(A)	w
49.	628.1	(A)	w
50.	596.0	(A)	w

51.	568.3	(A)	w
52.	490.3	(A)	w
53.	350.1	(A)	w
54.	320.0	(A)	w
55.	222.7	(A)	w
56.	82.5	(A)	vw
57.	79.2	(A)	vw
58.	(.0)	(t/r)	
59.	(.0)	(t/r)	
60.	(.0)	(t/r)	
61.	(.0)	(t/r)	
62.	(.0)	(t/r)	
63.	(.0)	(t/r)	

=====

STATISTICAL THERMODYNAMICS ANALYSIS

=====

Structure name : pyrrolizidine
 Temperature : 298.16 K
 Symmetry number : 1
 Optical isomers : 2
 Zero Point Energy : 116.798 Kcal/mol

	ENERGY (Kcal/mol)	ENTHALPY (Kcal/mol)	ENTROPY (eu)	FREE ENERGY (Kcal/mol)	HEAT CAPACITY (cal/mol/deg)
Translational	.889	1.481	40.014	-10.449	4.967
Rotational	.889	.889	27.716	-7.375	2.980
Vibrational	119.648%	119.648%	16.764*	114.650%	23.293*
Potential	39.487#	39.487#	.000	39.487#	.000
Mixing	.000	.000	1.377	-.411	.000
Total	160.912	161.505	85.870	135.902	31.241

Enthalpy Function (H-Ho)/T = 17.51 cal/mol/deg
 Free Energy Function -(G-Ho)/T = 68.36 cal/mol/deg

% Includes zero point energy (ZPE).
 * Excludes contribution from frequencies lower than 40 (1/cm).
 # Includes steric energy (SE).
 Internal rotation contributions are not considered

This structure has 0 imaginary frequencies,
 0 free internal rotation (fir) frequencies
 (>= 0, < 10 /cm),
 0 restricted internal rotation (rir) frequencies
 (>= 10, < 40 /cm),
 6 zero frequencies, and
 57 real frequencies.

FINAL STERIC ENERGY IS 39.4867 KCAL/MOL.

COMPRESSION	1.1986
BENDING	7.8017
BEND-BEND	.2857
STRETCH-BEND	-.3707
VANDERWAALS	
1,4 ENERGY	6.4009
OTHER	-.0453

TORSIONAL	24.9729
TORSION-STRETCH	-.7570
DIPOLE-DIPOLE	.0000
CHARGE-DIPOLE	.0000
CHARGE-CHARGE	.0000

COORDINATES TRANSLATED TO NEW ORIGIN WHICH IS CENTER OF MASS

C(1)	-.90683	1.25960	.45808	(1)
C(2)	.10173	.79027	-.61072	(1)
N(3)	-.06504	-.66581	-.60314	(8)
C(4)	-1.48996	-.95679	-.42798	(1)
C(5)	-2.01640	.17744	.47786	(1)
C(6)	1.58753	.98858	-.24274	(1)
C(7)	.76956	-1.20161	.47514	(1)
C(8)	2.05073	-.35931	.37005	(1)
H(9)	-.42393	1.32513	1.45896	(5)
H(10)	-1.31436	2.26562	.21428	(5)
H(11)	-.15278	1.20164	-1.61297	(5)
H(12)	-1.99489	-.91313	-1.41913	(5)
H(13)	-1.65891	-1.97084	-.00266	(5)
H(14)	-2.18866	-.18731	1.51556	(5)
H(15)	-2.98034	.57805	.09164	(5)
H(16)	2.18673	1.22033	-1.15227	(5)
H(17)	1.71676	1.83210	.47049	(5)
H(18)	.28637	-1.04909	1.47833	(5)
H(19)	.96171	-2.28741	.33456	(5)
H(20)	2.53632	-.22302	1.36163	(5)
H(21)	2.78244	-.85453	-.30836	(5)

MOMENT OF INERTIA WITH THE PRINCIPAL AXES

(1) UNIT = 10**(-39) GM*CM**2
 IX= 22.8107 IY= 42.5052 IZ= 52.9976

(2) UNIT = AU A**2
 IX= 137.3846 IY= 256.0005 IZ= 319.1940

DIPOLE MOMENT = .677 D

COMPONENTS WITH PRINCIPAL AXES

X = .1967 Y = -.2918 Z = -.5783

Pyrrolizidine 4 (cis-conformer)CONFORMATIONAL ENERGY, PART 3: GEOMETRY AND STERIC ENERGY
OF FINAL CONFORMATION.

CONNECTED ATOMS

1- 2- 3- 4- 5- 1-
 2- 6- 8- 7-
 3- 7-

ATTACHED ATOMS

1- 9, 1- 10, 2- 11, 4- 12, 4- 13, 5- 14, 5- 15,
 6- 16, 6- 17, 7- 18, 7- 19, 8- 20, 8- 21,

FINAL ATOMIC COORDINATE

ATOM	X	Y	Z	TYPE
C(1)	-.90683	1.25960	.45808	(1)
C(2)	.10173	.79027	-.61072	(1)
N(3)	-.06504	-.66581	-.60314	(8)
C(4)	-1.48996	-.95679	-.42798	(1)
C(5)	-2.01640	.17744	.47786	(1)
C(6)	1.58753	.98858	-.24274	(1)
C(7)	.76956	-1.20161	.47514	(1)
C(8)	2.05073	-.35931	.37005	(1)
H(9)	-.42393	1.32513	1.45896	(5)
H(10)	-1.31436	2.26562	.21428	(5)
H(11)	-.15278	1.20164	-1.61297	(5)
H(12)	-1.99489	-.91313	-1.41913	(5)
H(13)	-1.65891	-1.97084	-.00266	(5)
H(14)	-2.18866	-.18731	1.51556	(5)
H(15)	-2.98034	.57805	.09164	(5)
H(16)	2.18673	1.22033	-1.15227	(5)
H(17)	1.71676	1.83210	.47049	(5)
H(18)	.28637	-1.04909	1.47833	(5)
H(19)	.96171	-2.28741	.33456	(5)
H(20)	2.53632	-.22302	1.36163	(5)
H(21)	2.78244	-.85453	-.30836	(5)

THIS MOLECULE CONTAINS

2 5-MEMBERED RING(S)

DIELECTRIC CONSTANT = 1.500

BOND LENGTHS AND STRETCHING ENERGY (22 BONDS)

ENERGY = 71.94(KS)(DR)(DR)(1-(CS)(DR)+(7/12)((CS)(DR))**2)
 DR = R-RO
 CS = 2.550

BOND	LENGTH	R(0)	K(S)	R(0)-CORR ENERGY	CORR E-NEG	MISCEL	KS
C(1)- C(2)	1.5427	1.5208	4.490	.1460	-.0050		
C(1)- C(5)	1.5500	1.5226	4.490	.2274	-.0032		
C(1)- H(9)	1.1132	1.1116	4.694	.0009	-.0004	.014	
C(1)- H(10)	1.1125	1.1116	4.694	.0003	-.0004	.014	
C(2)- N(3)	1.4656	1.4530	5.300	.0588			
C(2)- C(6)	1.5435	1.5208	4.490	.1569	-.0050		
C(2)- H(11)	1.1129	1.1114	4.831	.0008	-.0011	.0005 BH	.021
N(3)- C(4)	1.4648	1.4530	5.300	.0518			
N(3)- C(7)	1.4650	1.4530	5.300	.0536			
C(4)- C(5)	1.5441	1.5208	4.490	.1650	-.0050		
C(4)- H(12)	1.1132	1.1114	4.701	.0012	-.0011	.0005 BH	.021
C(4)- H(13)	1.1125	1.1124	4.666	.0000	-.0011	.0015 BH	.014
C(5)- H(14)	1.1133	1.1116	4.694	.0011	-.0004	.014	
C(5)- H(15)	1.1130	1.1116	4.694	.0007	-.0004	.014	
C(6)- C(8)	1.5514	1.5226	4.490	.2500	-.0032		
C(6)- H(16)	1.1136	1.1116	4.694	.0013	-.0004	.014	
C(6)- H(17)	1.1122	1.1116	4.694	.0001	-.0004	.014	
C(7)- C(8)	1.5368	1.5208	4.490	.0799	-.0050		

```

C( 7)- H( 18) 1.1239 1.1225 4.337 .0006 -.0011 .0116 BH -.343
C( 7)- H( 19) 1.1116 1.1113 4.702 .0000 -.0011 .0004 BH .022
C( 8)- H( 20) 1.1125 1.1116 4.694 .0003 -.0004 .014
C( 8)- H( 21) 1.1139 1.1116 4.694 .0019 -.0004 .014

```

NON-BONDED DISTANCES, VDW AND EPR ENERGY (143 PAIRS)

```

E(VDW) = KV*(1.84(10**5)EXP(-12.00/P) - 2.25(P**6))
E(EPR) = C*KV*(1.84(10**5)EXP(-12.00/Q) - 2.25(Q**6))
E(HBD) = EP1-EP2*COS(THETA)*RTH/RTH0
          EP1 = KHB*1.84(10**5)*EXP(-12.0/P)
          EP2 = KHB*2.25(P**6)

```

```

IF P > 3.020, THEN,
E(VDW) = KV(192.270)/(P**2)
E(HBD) = EP1-EP2*COS(THETA)*RTH/RTH0
          EP1 = KHB*(192.270*P**2+1706.96)
          EP2 = KHB*1706.96

```

```

WHERE RV = RVDW(I) + RVDW(K)
      KV = SQRT(EPS(I)*EPS(K))
      KHB = EPS/DIELEC FOR HYDROGEN BOND
      P = (RV/R) OR (RV/R#)
      C = SCALE FACTOR
      Q = RV/R, WHERE R IS MODIFIED DISTANCE
      THETA = ANGLE H-X-Y IN HYDROGEN BOND X-H...Y
      RTH = BOND LENGTH X-H IN X-H...Y
      RTH0 = NATURAL BOND LENGTH X-H

```

IN THE VDW CALCULATIONS THE HYDROGEN ATOMS ARE RELOCATED
SO THAT THE ATTACHED HYDROGEN DISTANCE IS REDUCED BY .923

IN THE VDW CALCULATIONS THE DEUTERIUM ATOMS ARE RELOCATED
SO THAT THE ATTACHED DEUTERIUM DISTANCE IS REDUCED BY .923

** INTERACTIONS OF LESS THAN 0.1 KCAL/MOL ARE NOT PRINTED **

ATOM PAIR	R	R#	RV	KV	ENERGY
C(1), C(7)	2.9779		4.080	.0270	.3787 1,4
C(1), H(17)	2.6854	2.6628	3.560	.0230	.2396 1,4
C(1), H(18)	2.7919	2.7906	3.560	.0230	.1247
C(2), H(12)	2.8197	2.7719	3.560	.0230	.1382 1,4
C(2), H(18)	2.7895	2.7428	3.560	.0230	.1612 1,4
N(3), H(9)	2.8888	2.8357	3.550	.0293	.1168 1,4
N(3), H(21)	2.8689	2.8167	3.550	.0293	.1310 1,4
C(4), H(11)	2.8020	2.7552	3.560	.0230	.1511 1,4
C(4), H(18)	2.6073	2.5778	3.560	.0230	.3536 1,4
C(5), C(7)	3.1086		4.080	.0270	.2209 1,4
C(5), H(18)	2.7943	2.8038	3.560	.0230	.1159
C(6), H(9)	2.6561	2.6356	3.560	.0230	.2722 1,4
C(7), H(13)	2.5918	2.5637	3.560	.0230	.3762 1,4
H(9), H(14)	2.3249	2.2650	3.240	.0200	.4513 1,4
H(9), H(17)	2.4118	2.4153	3.240	.0200	.2174
H(9), H(18)	2.4783	2.5070	3.240	.0200	.1318
H(10), H(11)	2.4125	2.3426	3.240	.0200	.3128 1,4
H(10), H(15)	2.3745	2.3108	3.240	.0200	.3643 1,4
H(11), H(16)	2.3845	2.3188	3.240	.0200	.3507 1,4
H(12), H(15)	2.3403	2.2779	3.240	.0200	.4250 1,4
H(13), H(14)	2.4014	2.3344	3.240	.0200	.3254 1,4
H(16), H(21)	2.3178	2.2586	3.240	.0200	.4647 1,4
H(17), H(20)	2.3852	2.3209	3.240	.0200	.3472 1,4
H(18), H(20)	2.3996	2.3302	3.240	.0200	.3320 1,4
H(19), H(21)	2.4045	2.3350	3.240	.0200	.3245 1,4

BOND ANGLES, BENDING AND STRETCH-BEND ENERGIES (45 ANGLES)

```

EB = 0.021914(KB)(DT)(DT)(1+CF*DT+QF*DT**2+PF*DT**3+SF*DT**4)
      DT = THETA-TZERO
      CF = -1400.000E-5

```

QF = 5.600E-5
 PF = -.070E-5
 SF = .022E-6
 ESB(J) = 2.51124(KSB(J))(DT)(DR1+DR2)
 DR(I) = R(I) - R0(I)
 EBDDBD = -0.02191418(KBB1)(DT1)(KBB2)(DT2)

A T O M S				THETA	TZERO	KB	EB	KSB	ESB
C(2)-C(1)-C(5)	105.334	111.000	.670	.5097	.13	-.0912			
C(2)-C(1)-H(9)	110.930	109.310	.590	.0332	.08	.0076			
C(2)-C(1)-H(10)	111.271	109.310	.590	.0484	.08	.0090			
C(5)-C(1)-H(9)	109.886	109.310	.590	.0043	.08	.0034			
C(5)-C(1)-H(10)	111.833	109.310	.590	.0794	.08	.0144			
H(9)-C(1)-H(10)	107.621	107.600	.550	.0000					
C(1)-C(2)-N(3)	102.960	108.000	.780	.4654	.13	-.0567			
C(1)-C(2)-C(6)	115.156	110.200	.670	.3361	.13	.0721			
C(1)-C(2)-H(11)	111.222	109.800	.590	.0256	.08	.0067			
N(3)-C(2)-C(6)	103.647	108.000	.780	.3440	.13	-.0502			
N(3)-C(2)-H(11)	110.235	109.300	.820	.0155	.08	.0027			
C(6)-C(2)-H(11)	112.791	109.800	.590	.1108	.08	.0145			
C(2)-N(3)-C(4)	107.978	114.000	.720	.6217	.10	-.0370			
C(2)-N(3)-C(7)	107.598	114.000	.720	.7063	.10	-.0396			
C(4)-N(3)-C(7)	113.172	107.200	.720	.5167	.05	.0179			
N(3)-C(4)-C(5)	104.826	109.700	.780	.4343	.13	-.0559			
N(3)-C(4)-H(12)	109.085	109.300	.820	.0008	.08	-.0006			
N(3)-C(4)-H(13)	111.993	109.300	.820	.1255	.08	.0065			
C(5)-C(4)-H(12)	109.808	109.310	.590	.0032	.08	.0025			
C(5)-C(4)-H(13)	113.172	109.310	.590	.1826	.08	.0181			
H(12)-C(4)-H(13)	107.893	107.600	.550	.0010					
C(1)-C(5)-C(4)	105.147	111.000	.670	.5453	.13	-.0970			
C(1)-C(5)-H(14)	110.572	109.310	.590	.0202	.08	.0074			
C(1)-C(5)-H(15)	111.361	109.310	.590	.0528	.08	.0119			
C(4)-C(5)-H(14)	111.032	109.310	.590	.0374	.08	.0087			
C(4)-C(5)-H(15)	110.861	109.310	.590	.0304	.08	.0077			
H(14)-C(5)-H(15)	107.900	107.600	.550	.0011					
C(2)-C(6)-C(8)	105.661	111.000	.670	.4505	.13	-.0898			
C(2)-C(6)-H(16)	110.488	109.310	.590	.0176	.08	.0058			
C(2)-C(6)-H(17)	111.235	109.310	.590	.0466	.08	.0090			
C(8)-C(6)-H(16)	110.046	109.310	.590	.0069	.08	.0046			
C(8)-C(6)-H(17)	111.774	109.310	.590	.0758	.08	.0146			
H(16)-C(6)-H(17)	107.664	107.600	.550	.0000					
N(3)-C(7)-C(8)	102.952	109.700	.780	.8541	.13	-.0619			
N(3)-C(7)-H(18)	111.249	109.300	.820	.0664	.08	.0053			
N(3)-C(7)-H(19)	111.262	109.300	.820	.0673	.08	.0049			
C(8)-C(7)-H(18)	110.185	109.310	.590	.0098	.08	.0031			
C(8)-C(7)-H(19)	112.495	109.310	.590	.1254	.08	.0104			
H(18)-C(7)-H(19)	108.649	107.600	.550	.0131					
C(6)-C(8)-C(7)	104.731	111.000	.670	.6290	.13	-.0919			
C(6)-C(8)-H(20)	112.082	109.310	.590	.0956	.08	.0166			
C(6)-C(8)-H(21)	109.987	109.310	.590	.0059	.08	.0042			
C(7)-C(8)-H(20)	111.720	109.310	.590	.0726	.08	.0082			
C(7)-C(8)-H(21)	110.217	109.310	.590	.0105	.08	.0034			
H(20)-C(8)-H(21)	108.094	107.600	.550	.0029					

DIHEDRAL ANGLES, TORSIONAL ENERGY (ET) (72 ANGLES)

$$ET = (V1/2)(1+\cos(W)) + (V2/2)(1-\cos(2W)) + (V3/2)(1+\cos(3W))$$

$$ETS = -11.995*(R-R0)((KTS1/2)(1+\cos(W)) + (KTS2/2)(1-\cos(2W)) + (KTS3/2)(1+\cos(3W)))$$

SIGN OF ANGLE A-B-C-D : WHEN LOOKING THROUGH B TOWARD C,
IF D IS COUNTERCLOCKWISE FROM A, NEGATIVE.

A T O M S				OMEGA	V1	V2	V3	ET	KTS3	ETS
C(1)C(2)N(3)C(4)	38.3	.958	-.155	1.360	1.190	.061	-.003			
C(1)C(2)N(3)C(7)	-84.2	.958	-.155	.766	.642	.061	-.003			
C(1)C(2)C(6)C(8)	94.7	.185	.170	.520	.577	.059	-.010			
C(1)C(2)C(6)H(16)	-146.3	.000	.000	.280	.167	.059	-.010			

C(1) C(2) C(6) H(17) -26.8 .000 .000 .280 .163 .059 -.009
C(1) C(5) C(4) N(3) 14.5 -.302 .696 1.360 .920 .059 -.014
C(1) C(5) C(4) H(12) -102.6 .000 .000 .280 .226 .059 -.013
C(1) C(5) C(4) H(13) 136.8 .000 .000 .280 .229 .059 -.013
C(2) C(1) C(5) C(4) 8.0 .185 .170 1.160 1.298 .059 -.019
C(2) C(1) C(5) H(14) 127.9 .000 .000 .280 .268 .059 -.019
C(2) C(1) C(5) H(15) -112.2 .000 .000 .280 .268 .059 -.019
C(2) N(3) C(4) C(5) -33.5 .958 -.155 1.360 1.388 .061 -.004
C(2) N(3) C(4) H(12) 84.1 .072 -.012 .563 .223 .061 -.003
C(2) N(3) C(4) H(13) -156.6 .072 -.012 .563 .188 .061 -.003
C(2) N(3) C(7) C(8) -40.4 .958 -.155 1.360 1.107 .061 -.002
C(2) N(3) C(7) H(18) 77.6 .072 -.012 .563 .144 .061 -.002
C(2) N(3) C(7) H(19) -161.1 .072 -.012 .563 .128 .061 -.002
C(2) C(6) C(8) C(7) -6.5 .185 .170 1.160 1.313 .059 -.020
C(2) C(6) C(8) H(20) -127.8 .000 .000 .280 .268 .059 -.020
C(2) C(6) C(8) H(21) 111.9 .000 .000 .280 .268 .059 -.020
N(3) C(2) C(1) C(5) -27.4 -.302 .696 1.360 .635 .059 -.009
N(3) C(2) C(1) H(9) 91.5 .000 .000 .374 .201 .059 -.008
N(3) C(2) C(1) H(10) -148.8 .000 .000 .374 .199 .059 -.008
N(3) C(2) C(6) C(8) -17.0 -.302 .696 1.360 .873 .059 -.013
N(3) C(2) C(6) H(16) 102.0 .000 .000 .374 .297 .059 -.013
N(3) C(2) C(6) H(17) -138.5 .000 .000 .374 .293 .059 -.013
N(3) C(4) C(5) H(14) -105.1 .000 .000 .374 .320 .059 -.014
N(3) C(4) C(5) H(15) 135.0 .000 .000 .374 .319 .059 -.014
N(3) C(7) C(8) C(6) 27.6 -.302 .696 1.360 .631 .059 -.006
N(3) C(7) C(8) H(20) 149.1 .000 .000 .374 .196 .059 -.006
N(3) C(7) C(8) H(21) -90.7 .000 .000 .374 .194 .059 -.006
C(4) N(3) C(2) C(6) 158.6 .958 -.155 .766 .229 .061 -.003
C(4) N(3) C(2) H(11) -80.4 .072 -.012 .563 .177 .061 -.002
C(4) N(3) C(7) C(8) -159.6 .958 -.155 .766 .210 .061 -.002
C(4) N(3) C(7) H(18) -41.6 .072 -.012 .563 .178 .061 -.002
C(4) N(3) C(7) H(19) 79.7 .072 -.012 .563 .168 .061 -.002
C(4) C(5) C(1) H(9) -111.6 .000 .000 .280 .267 .059 -.019
C(4) C(5) C(1) H(10) 129.0 .000 .000 .280 .265 .059 -.018
C(5) C(1) C(2) C(6) -139.5 .185 .170 .520 .490 .059 -.012
C(5) C(1) C(2) H(11) 90.6 .000 .000 .280 .145 .059 -.008
C(5) C(4) N(3) C(7) 85.5 .958 -.155 .766 .656 .061 -.003
C(6) C(2) C(1) H(9) -20.6 .000 .000 .280 .206 .059 -.011
C(6) C(2) C(1) H(10) 99.2 .000 .000 .280 .205 .059 -.011
C(6) C(2) N(3) C(7) 36.1 .958 -.155 1.360 1.278 .061 -.003
C(6) C(8) C(7) H(18) -91.2 .000 .000 .280 .149 .059 -.006
C(6) C(8) C(7) H(19) 147.4 .000 .000 .280 .159 .059 -.006
C(7) N(3) C(2) H(11) 157.1 .072 -.012 .563 .181 .061 -.003
C(7) N(3) C(4) H(12) -156.9 .072 -.012 .563 .182 .061 -.003
C(7) N(3) C(4) H(13) -37.6 .072 -.012 .563 .233 .061 -.003
C(7) C(8) C(6) H(16) -125.8 .000 .000 .280 .274 .059 -.020
C(7) C(8) C(6) H(17) 114.6 .000 .000 .280 .275 .059 -.020
C(8) C(6) C(2) H(11) -136.2 .000 .000 .280 .233 .059 -.013
H(9) C(1) C(2) H(11) -150.5 .000 .000 .238 .116 .059 -.008
H(9) C(1) C(5) H(14) 8.3 .000 .000 .238 .227 .059 -.019
H(9) C(1) C(5) H(15) 128.3 .000 .000 .238 .227 .059 -.019
H(10) C(1) C(2) H(11) -30.7 .000 .000 .238 .114 .059 -.007
H(10) C(1) C(5) H(14) -111.1 .000 .000 .238 .225 .059 -.018
H(10) C(1) C(5) H(15) 8.8 .000 .000 .238 .226 .059 -.018
H(11) C(2) C(6) H(16) -17.2 .000 .000 .238 .193 .059 -.013
H(11) C(2) C(6) H(17) 102.3 .000 .000 .238 .191 .059 -.013
H(12) C(4) C(5) H(14) 137.8 .000 .000 .238 .190 .059 -.013
H(12) C(4) C(5) H(15) 17.9 .000 .000 .238 .189 .059 -.013
H(13) C(4) C(5) H(14) 17.2 .000 .000 .238 .193 .059 -.013
H(13) C(4) C(5) H(15) -102.7 .000 .000 .238 .193 .059 -.013
H(16) C(6) C(8) H(20) 112.9 .000 .000 .238 .230 .059 -.020
H(16) C(6) C(8) H(21) -7.4 .000 .000 .238 .229 .059 -.020
H(17) C(6) C(8) H(20) -6.7 .000 .000 .238 .231 .059 -.020
H(17) C(6) C(8) H(21) -127.0 .000 .000 .238 .230 .059 -.020
H(18) C(7) C(8) H(20) 30.4 .000 .000 .238 .117 .059 -.006
H(18) C(7) C(8) H(21) 150.6 .000 .000 .238 .115 .059 -.006
H(19) C(7) C(8) H(20) -91.0 .000 .000 .238 .125 .059 -.006
H(19) C(7) C(8) H(21) 29.2 .000 .000 .238 .124 .059 -.006

=====

NORMAL MODE VIBRATIONAL ANALYSIS

Molecular Shape : ASYMMETRIC ROTOR WITH KAPPA = -.626937
 Symmetry Point Group : C1
 Symmetry Number : 1
 Chirality : yes

0 FUNDAMENTAL NORMAL VIBRATIONAL FREQUENCIES
(THEORETICALLY 57 VALUES)

Frequency : in 1/cm
 A(i) : IR intensity (vs,s,m,w,vw,-- or in 10**6 cm/mole)
 A(i) = -- : IR inactive

no	Frequency	Symmetry	A(i)
1.	2958.6	(A)	m
2.	2947.7	(A)	s
3.	2947.4	(A)	m
4.	2945.6	(A)	w
5.	2942.1	(A)	w
6.	2939.9	(A)	w
7.	2938.8	(A)	m
8.	2896.1	(A)	m
9.	2892.6	(A)	m
10.	2889.0	(A)	m
11.	2880.8	(A)	m
12.	2879.7	(A)	w
13.	2797.6	(A)	m
14.	1503.0	(A)	w
15.	1471.2	(A)	w
16.	1427.2	(A)	w
17.	1417.1	(A)	w
18.	1408.6	(A)	w
19.	1408.1	(A)	w
20.	1394.3	(A)	w
21.	1386.7	(A)	w
22.	1363.3	(A)	w
23.	1357.1	(A)	w
24.	1322.4	(A)	w
25.	1317.6	(A)	w
26.	1303.2	(A)	w
27.	1281.9	(A)	w
28.	1268.4	(A)	w
29.	1246.9	(A)	w
30.	1186.9	(A)	w
31.	1171.3	(A)	w
32.	1168.6	(A)	w
33.	1137.2	(A)	w
34.	1119.7	(A)	w
35.	1107.9	(A)	w
36.	1035.8	(A)	w
37.	1012.7	(A)	w
38.	1006.3	(A)	vw
39.	973.3	(A)	w
40.	962.3	(A)	w
41.	943.4	(A)	w
42.	899.6	(A)	w
43.	883.2	(A)	w
44.	857.9	(A)	w
45.	843.4	(A)	w
46.	798.6	(A)	w
47.	765.2	(A)	w
48.	759.7	(A)	w
49.	628.1	(A)	w
50.	596.0	(A)	w

51.	568.3	(A)	w
52.	490.3	(A)	w
53.	350.1	(A)	w
54.	320.0	(A)	w
55.	222.7	(A)	w
56.	82.5	(A)	vw
57.	79.2	(A)	vw
58.	(.0)	(t/r)	
59.	(.0)	(t/r)	
60.	(.0)	(t/r)	
61.	(.0)	(t/r)	
62.	(.0)	(t/r)	
63.	(.0)	(t/r)	

=====

STATISTICAL THERMODYNAMICS ANALYSIS

=====

Structure name : pyrrolizidine
 Temperature : 298.16 K
 Symmetry number : 1
 Optical isomers : 2
 Zero Point Energy : 116.798 Kcal/mol

	ENERGY (Kcal/mol)	ENTHALPY (Kcal/mol)	ENTROPY (eu)	FREE ENERGY (Kcal/mol)	HEAT CAPACITY (cal/mol/deg)
Translational	.889	1.481	40.014	-10.449	4.967
Rotational	.889	.889	27.716	-7.375	2.980
Vibrational	119.648%	119.648%	16.764*	114.650%	23.293*
Potential	39.487#	39.487#	.000	39.487#	.000
Mixing	.000	.000	1.377	-.411	.000
Total	160.912	161.505	85.870	135.902	31.241

Enthalpy Function (H-Ho)/T = 17.51 cal/mol/deg
 Free Energy Function -(G-Ho)/T = 68.36 cal/mol/deg

% Includes zero point energy (ZPE).
 * Excludes contribution from frequencies lower than 40 (1/cm).
 # Includes steric energy (SE).
 Internal rotation contributions are not considered

This structure has 0 imaginary frequencies,
 0 free internal rotation (fir) frequencies
 (>= 0, < 10 /cm),
 0 restricted internal rotation (rir) frequencies
 (>= 10, < 40 /cm),
 6 zero frequencies, and
 57 real frequencies.

FINAL STERIC ENERGY IS 39.4867 KCAL/MOL.

COMPRESSION	1.1986
BENDING	7.8017
BEND-BEND	.2857
STRETCH-BEND	-.3707
VANDERWAALS	
1,4 ENERGY	6.4009
OTHER	-.0453

TORSIONAL	24.9729
TORSION-STRETCH	-.7570
DIPOLE-DIPOLE	.0000
CHARGE-DIPOLE	.0000
CHARGE-CHARGE	.0000

COORDINATES TRANSLATED TO NEW ORIGIN WHICH IS CENTER OF MASS

C(1)	-.90683	1.25960	.45808	(1)
C(2)	.10173	.79027	-.61072	(1)
N(3)	-.06504	-.66581	-.60314	(8)
C(4)	-1.48996	-.95679	-.42798	(1)
C(5)	-2.01640	.17744	.47786	(1)
C(6)	1.58753	.98858	-.24274	(1)
C(7)	.76956	-1.20161	.47514	(1)
C(8)	2.05073	-.35931	.37005	(1)
H(9)	-.42393	1.32513	1.45896	(5)
H(10)	-1.31436	2.26562	.21428	(5)
H(11)	-.15278	1.20164	-1.61297	(5)
H(12)	-1.99489	-.91313	-1.41913	(5)
H(13)	-1.65891	-1.97084	-.00266	(5)
H(14)	-2.18866	-.18731	1.51556	(5)
H(15)	-2.98034	.57805	.09164	(5)
H(16)	2.18673	1.22033	-1.15227	(5)
H(17)	1.71676	1.83210	.47049	(5)
H(18)	.28637	-1.04909	1.47833	(5)
H(19)	.96171	-2.28741	.33456	(5)
H(20)	2.53632	-.22302	1.36163	(5)
H(21)	2.78244	-.85453	-.30836	(5)

MOMENT OF INERTIA WITH THE PRINCIPAL AXES

(1) UNIT = $10^{(-39)}$ GM*CM**2
 IX= 22.8107 IY= 42.5052 IZ= 52.9976

(2) UNIT = AU A**2
 IX= 137.3846 IY= 256.0005 IZ= 319.1940

DIPOLE MOMENT = .677 D

COMPONENTS WITH PRINCIPAL AXES

X = .1967 Y = -.2918 Z = -.5783

Pyrrolizidine 4 (trans-conformer)CONFORMATIONAL ENERGY, PART 3: GEOMETRY AND STERIC ENERGY
OF FINAL CONFORMATION.

CONNECTED ATOMS

1- 2- 3- 4- 5- 1-
 2- 6- 8- 7-
 3- 7-

ATTACHED ATOMS

1- 9, 1- 10, 2- 11, 4- 12, 4- 13, 5- 14, 5- 15,
 6- 16, 6- 17, 7- 18, 7- 19, 8- 20, 8- 21,

FINAL ATOMIC COORDINATE

ATOM	X	Y	Z	TYPE
C(1)	-1.34454	-1.23899	-.09466	(1)
C(2)	.00000	-.71456	.40945	(1)
N(3)	.00000	.60586	-.18942	(8)
C(4)	-1.28984	1.23513	.04343	(1)
C(5)	-2.25962	.02451	-.07102	(1)
C(6)	1.34454	-1.23899	-.09466	(1)
C(7)	1.28984	1.23513	.04343	(1)
C(8)	2.25963	.02451	-.07102	(1)
H(9)	-1.24741	-1.62094	-1.13606	(5)
H(10)	-1.73855	-2.05968	.54379	(5)
H(11)	.00000	-.62108	1.53278	(5)
H(12)	-1.32978	1.68510	1.07215	(5)
H(13)	-1.49401	2.02377	-.71276	(5)
H(14)	-2.87162	.08358	-.99893	(5)
H(15)	-2.95318	-.00206	.79937	(5)
H(16)	1.73855	-2.05968	.54379	(5)
H(17)	1.24741	-1.62094	-1.13606	(5)
H(18)	1.49401	2.02377	-.71276	(5)
H(19)	1.32978	1.68510	1.07215	(5)
H(20)	2.95318	-.00206	.79937	(5)
H(21)	2.87162	.08358	-.99893	(5)

THIS MOLECULE CONTAINS

2 5-MEMBERED RING(S)

DIELECTRIC CONSTANT = 1.500

BOND LENGTHS AND STRETCHING ENERGY (22 BONDS)

ENERGY = 71.94(KS)(DR)(DR)(1-(CS)(DR)+(7/12)((CS)(DR))**2)
 DR = R-RO
 CS = 2.550

BOND	LENGTH	R(0)	K(S)	R(0)-CORR ENERGY	CORR E-NEG	MISCEL	KS
C(1)- C(2)	1.5287	1.5208	4.490	.0198	-.0050		
C(1)- C(5)	1.5603	1.5226	4.490	.4173	-.0032		
C(1)- H(9)	1.1135	1.1116	4.694	.0012	-.0004	.014	
C(1)- H(10)	1.1119	1.1116	4.694	.0000	-.0004	.014	
C(2)- N(3)	1.4499	1.4530	5.300	.0037			
C(2)- C(6)	1.5287	1.5208	4.490	.0198	-.0050		
C(2)- H(11)	1.1272	1.1235	4.434	.0043	-.0011	.0126 BH	-.376
N(3)- C(4)	1.4539	1.4530	5.300	.0003			
N(3)- C(7)	1.4539	1.4530	5.300	.0003			
C(4)- C(5)	1.5554	1.5208	4.490	.3537	-.0050		
C(4)- H(12)	1.1235	1.1221	4.351	.0007	-.0011	.0112 BH	-.329
C(4)- H(13)	1.1115	1.1117	4.690	.0000	-.0011	.0008 BH	.010
C(5)- H(14)	1.1131	1.1116	4.694	.0008	-.0004	.014	
C(5)- H(15)	1.1132	1.1116	4.694	.0009	-.0004	.014	
C(6)- C(8)	1.5603	1.5226	4.490	.4173	-.0032		
C(6)- H(16)	1.1119	1.1116	4.694	.0000	-.0004	.014	
C(6)- H(17)	1.1135	1.1116	4.694	.0012	-.0004	.014	

S45

```

C( 7)- C( 8) 1.5554 1.5208 4.490 .3537 -.0050
C( 7)- H( 18) 1.1115 1.1117 4.690 .0000 -.0011 .0008 BH .010
C( 7)- H( 19) 1.1235 1.1221 4.351 .0006 -.0011 .0112 BH -.329
C( 8)- H( 20) 1.1132 1.1116 4.694 .0009 -.0004 .014
C( 8)- H( 21) 1.1131 1.1116 4.694 .0008 -.0004 .014

```

NON-BONDED DISTANCES, VDW AND EPR ENERGY (143 PAIRS)

```

E(VDW) = KV*(1.84(10**5)EXP(-12.00/P) - 2.25(P**6))
E(EPR) = C*KV*(1.84(10**5)EXP(-12.00/Q) - 2.25(Q**6))
E(HBD) = EP1-EP2*COS(THETA)*RTH/RTH0
EP1 = KHB*1.84(10**5)*EXP(-12.0/P)
EP2 = KHB*2.25(P**6)

```

IF P > 3.020, THEN,

```

E(VDW) = KV(192.270)(P**2)
E(HBD) = EP1-EP2*COS(THETA)*RTH/RTH0
EP1 = KHB*(192.270*P**2+1706.96)
EP2 = KHB*1706.96

```

WHERE RV = RVDW(I) + RVDW(K)

KV = SQRT(EPS(I)*EPS(K))

KHB = EPS/DIELEC FOR HYDROGEN BOND

P = (RV/R) OR (RV/R#)

C = SCALE FACTOR

Q = RV/R, WHERE R IS MODIFIED DISTANCE

THETA = ANGLE H-X-Y IN HYDROGEN BOND X-H...Y

RTH = BOND LENGTH X-H IN X-H...Y

RTH0 = NATURAL BOND LENGTH X-H

IN THE VDW CALCULATIONS THE HYDROGEN ATOMS ARE RELOCATED
SO THAT THE ATTACHED HYDROGEN DISTANCE IS REDUCED BY .923

IN THE VDW CALCULATIONS THE DEUTERIUM ATOMS ARE RELOCATED
SO THAT THE ATTACHED DEUTERIUM DISTANCE IS REDUCED BY .923

** INTERACTIONS OF LESS THAN 0.1 KCAL/MOL ARE NOT PRINTED **

ATOM PAIR	R	R#	RV	KV	ENERGY
C(1), H(17)	2.8193	2.7938	3.560	.0230	.1226 1,4
C(2), H(12)	2.8224	2.7738	3.560	.0230	.1368 1,4
C(2), H(19)	2.8224	2.7738	3.560	.0230	.1368 1,4
N(3), H(9)	2.7223	2.6747	3.550	.0293	.2783 1,4
N(3), H(17)	2.7223	2.6747	3.550	.0293	.2783 1,4
C(4), H(11)	2.7069	2.6653	3.560	.0230	.2367 1,4
C(4), H(19)	2.8501	2.8143	3.560	.0230	.1091 1,4
C(5), H(11)	2.8451	2.7990	3.560	.0230	.1190 1,4
C(6), H(9)	2.8193	2.7938	3.560	.0230	.1226 1,4
C(7), H(11)	2.7069	2.6653	3.560	.0230	.2367 1,4
C(7), H(12)	2.8501	2.8143	3.560	.0230	.1091 1,4
C(8), H(11)	2.8451	2.7990	3.560	.0230	.1190 1,4
H(9), H(14)	2.3584	2.2958	3.240	.0200	.3909 1,4
H(9), H(17)	2.4948	2.5098	3.240	.0200	.1297
H(10), H(11)	2.4638	2.3865	3.240	.0200	.2517 1,4
H(10), H(15)	2.4030	2.3371	3.240	.0200	.3211 1,4
H(11), H(16)	2.4638	2.3865	3.240	.0200	.2517 1,4
H(12), H(15)	2.3572	2.2949	3.240	.0200	.3927 1,4
H(13), H(14)	2.3967	2.3316	3.240	.0200	.3299 1,4
H(16), H(20)	2.4030	2.3371	3.240	.0200	.3211 1,4
H(17), H(21)	2.3584	2.2958	3.240	.0200	.3909 1,4
H(18), H(21)	2.3967	2.3316	3.240	.0200	.3299 1,4
H(19), H(20)	2.3572	2.2949	3.240	.0200	.3927 1,4

BOND ANGLES, BENDING AND STRETCH-BEND ENERGIES (45 ANGLES)

```

EB = 0.021914(KB)(DT)(DT)(1+CF*DT+QF*DT**2+PF*DT**3+SF*DT**4)
DT = THETA-TZERO
CF = -1400.000E-5
QF = 5.600E-5

```

S46

PF = -.070E-5
 SF = .022E-6
 ESB(J) = 2.51124(KSB(J))(DT)(DR1+DR2)
 DR(I) = R(I) - R0(I)
 EBDDBD = -0.02191418(KBB1)(DT1)(KBB2)(DT2)

A T O M S			THETA	TZERO	KB	EB	KSB	ESB
C(2)- C(1)- C(5)	103.476	111.000	.670	.9218	.13	-.1120		
C(2)- C(1)- H(9)	110.449	109.310	.590	.0165	.08	.0022		
C(2)- C(1)- H(10)	112.056	109.310	.590	.0938	.08	.0046		
C(5)- C(1)- H(9)	110.067	109.310	.590	.0073	.08	.0060		
C(5)- C(1)- H(10)	112.406	109.310	.590	.1187	.08	.0237		
H(9)- C(1)- H(10)	108.346	107.600	.550	.0066				
C(1)- C(2)- N(3)	100.149	108.000	.780	1.1733	.13	-.0123		
C(1)- C(2)- C(6)	123.171	110.200	.670	2.0427	.13	.0670		
C(1)- C(2)- H(11)	110.921	109.800	.590	.0160	.08	.0026		
N(3)- C(2)- C(6)	100.149	108.000	.780	1.1733	.13	-.0123		
N(3)- C(2)- H(11)	109.639	109.300	.820	.0021	.08	.0000		
C(6)- C(2)- H(11)	110.921	109.800	.590	.0160	.08	.0026		
C(2)- N(3)- C(4)	109.148	114.000	.720	.3972	.10	.0027		
C(2)- N(3)- C(7)	109.148	114.000	.720	.3972	.10	.0027		
C(4)- N(3)- C(7)	125.034	107.200	.720	3.8458	.05	.0041		
N(3)- C(4)- C(5)	101.799	109.700	.780	1.1892	.13	-.0915		
N(3)- C(4)- H(12)	110.580	109.300	.820	.0289	.08	.0006		
N(3)- C(4)- H(13)	111.167	109.300	.820	.0610	.08	.0003		
C(5)- C(4)- H(12)	110.912	109.310	.590	.0324	.08	.0116		
C(5)- C(4)- H(13)	112.809	109.310	.590	.1507	.08	.0242		
H(12)- C(4)- H(13)	109.404	107.600	.550	.0382				
C(1)- C(5)- C(4)	105.411	111.000	.670	.4954	.13	-.1318		
C(1)- C(5)- H(14)	110.658	109.310	.590	.0231	.08	.0106		
C(1)- C(5)- H(15)	110.972	109.310	.590	.0349	.08	.0131		
C(4)- C(5)- H(14)	111.275	109.310	.590	.0485	.08	.0143		
C(4)- C(5)- H(15)	110.457	109.310	.590	.0167	.08	.0084		
H(14)- C(5)- H(15)	108.089	107.600	.550	.0029				
C(2)- C(6)- C(8)	103.476	111.000	.670	.9218	.13	-.1120		
C(2)- C(6)- H(16)	112.056	109.310	.590	.0938	.08	.0046		
C(2)- C(6)- H(17)	110.449	109.310	.590	.0165	.08	.0022		
C(8)- C(6)- H(16)	112.406	109.310	.590	.1187	.08	.0237		
C(8)- C(6)- H(17)	110.067	109.310	.590	.0073	.08	.0060		
H(16)- C(6)- H(17)	108.346	107.600	.550	.0066				
N(3)- C(7)- C(8)	101.799	109.700	.780	1.1892	.13	-.0915		
N(3)- C(7)- H(18)	111.167	109.300	.820	.0610	.08	.0003		
N(3)- C(7)- H(19)	110.580	109.300	.820	.0289	.08	.0006		
C(8)- C(7)- H(18)	112.809	109.310	.590	.1507	.08	.0242		
C(8)- C(7)- H(19)	110.912	109.310	.590	.0324	.08	.0116		
H(18)- C(7)- H(19)	109.404	107.600	.550	.0382				
C(6)- C(8)- C(7)	105.411	111.000	.670	.4954	.13	-.1318		
C(6)- C(8)- H(20)	110.972	109.310	.590	.0349	.08	.0131		
C(6)- C(8)- H(21)	110.658	109.310	.590	.0231	.08	.0106		
C(7)- C(8)- H(20)	110.457	109.310	.590	.0167	.08	.0084		
C(7)- C(8)- H(21)	111.275	109.310	.590	.0485	.08	.0143		
H(20)- C(8)- H(21)	108.089	107.600	.550	.0029				

DIHEDRAL ANGLES, TORSIONAL ENERGY (ET) (72 ANGLES)

$$ET = (V1/2)(1+\cos(W)) + (V2/2)(1-\cos(2W)) + (V3/2)(1+\cos(3W))$$

$$ETS = -11.995 \cdot (R-R0) \cdot ((KTS1/2)(1+\cos(W)) + (KTS2/2)(1-\cos(2W)) + (KTS3/2)(1+\cos(3W)))$$

SIGN OF ANGLE A-B-C-D : WHEN LOOKING THROUGH B TOWARD C,
IF D IS COUNTERCLOCKWISE FROM A, NEGATIVE.

A T O M S			OMEGA	V1	V2	V3	ET	KTS3	ETS
C(1) C(2) N(3) C(4)	46.8	.958	-.155	1.360	.881	.061	.000		
C(1) C(2) N(3) C(7)	-173.4	.958	-.155	.766	.024	.061	.000		
C(1) C(2) C(6) C(8)	145.5	.185	.170	.520	.391	.059	-.003		
C(1) C(2) C(6) H(16)	-93.1	.000	.000	.280	.163	.059	-.003		
C(1) C(2) C(6) H(17)	27.8	.000	.000	.280	.156	.059	-.003		

C(1) C(5) C(4) N(3) 10.6 -.302 .696 1.360 .982 .059 -.023
C(1) C(5) C(4) H(12)-107.1 .000 .000 .280 .249 .059 -.022
C(1) C(5) C(4) H(13) 129.8 .000 .000 .280 .262 .059 -.023
C(2) C(1) C(5) C(4) 15.9 .185 .170 1.160 1.164 .059 -.022
C(2) C(1) C(5) H(14) 136.3 .000 .000 .280 .232 .059 -.022
C(2) C(1) C(5) H(15)-103.7 .000 .000 .280 .232 .059 -.022
C(2) N(3) C(4) C(5) -36.3 .958 -.155 1.360 1.272 .061 .000
C(2) N(3) C(4) H(12) 81.6 .072 -.012 .563 .192 .061 .000
C(2) N(3) C(4) H(13)-156.6 .072 -.012 .563 .187 .061 .000
C(2) N(3) C(7) C(8) 36.3 .958 -.155 1.360 1.272 .061 .000
C(2) N(3) C(7) H(18) 156.6 .072 -.012 .563 .187 .061 .000
C(2) N(3) C(7) H(19) -81.6 .072 -.012 .563 .192 .061 .000
C(2) C(6) C(8) C(7) -15.9 .185 .170 1.160 1.164 .059 -.022
C(2) C(6) C(8) H(20) 103.7 .000 .000 .280 .232 .059 -.022
C(2) C(6) C(8) H(21)-136.3 .000 .000 .280 .232 .059 -.022
N(3) C(2) C(1) C(5) -36.2 -.302 .696 1.360 .433 .059 -.002
N(3) C(2) C(1) H(9) 81.6 .000 .000 .374 .107 .059 -.002
N(3) C(2) C(1) H(10)-157.5 .000 .000 .374 .115 .059 -.002
N(3) C(2) C(6) C(8) 36.2 -.302 .696 1.360 .433 .059 -.002
N(3) C(2) C(6) H(16) 157.5 .000 .000 .374 .115 .059 -.002
N(3) C(2) C(6) H(17) -81.6 .000 .000 .374 .107 .059 -.002
N(3) C(4) C(5) H(14)-109.4 .000 .000 .374 .346 .059 -.023
N(3) C(4) C(5) H(15) 130.5 .000 .000 .374 .346 .059 -.023
N(3) C(7) C(8) C(6) -10.6 -.302 .696 1.360 .982 .059 -.023
N(3) C(7) C(8) H(20)-130.5 .000 .000 .374 .346 .059 -.023
N(3) C(7) C(8) H(21) 109.4 .000 .000 .374 .346 .059 -.023
C(4) N(3) C(2) C(6) 173.4 .958 -.155 .766 .024 .061 .000
C(4) N(3) C(2) H(11) -69.9 .072 -.012 .563 .075 .061 .000
C(4) N(3) C(7) C(8) 168.1 .958 -.155 .766 .075 .061 .000
C(4) N(3) C(7) H(18) -71.5 .072 -.012 .563 .086 .061 .000
C(4) N(3) C(7) H(19) 50.2 .072 -.012 .563 .088 .061 .000
C(4) C(5) C(1) H(9)-102.1 .000 .000 .280 .223 .059 -.021
C(4) C(5) C(1) H(10) 137.0 .000 .000 .280 .228 .059 -.022
C(5) C(1) C(2) C(6) -145.5 .185 .170 .520 .391 .059 -.003
C(5) C(1) C(2) H(11) 79.5 .000 .000 .280 .067 .059 -.001
C(5) C(4) N(3) C(7) -168.1 .958 -.155 .766 .075 .061 .000
C(6) C(2) C(1) H(9) -27.8 .000 .000 .280 .156 .059 -.003
C(6) C(2) C(1) H(10) 93.1 .000 .000 .280 .163 .059 -.003
C(6) C(2) N(3) C(7) -46.8 .958 -.155 1.360 .881 .061 .000
C(6) C(8) C(7) H(18)-129.8 .000 .000 .280 .262 .059 -.023
C(6) C(8) C(7) H(19) 107.1 .000 .000 .280 .249 .059 -.022
C(7) N(3) C(2) H(11) 69.9 .072 -.012 .563 .075 .061 .000
C(7) N(3) C(4) H(12) -50.2 .072 -.012 .563 .088 .061 .000
C(7) N(3) C(4) H(13) 71.5 .072 -.012 .563 .086 .061 .000
C(7) C(8) C(6) H(16)-137.0 .000 .000 .280 .228 .059 -.022
C(7) C(8) C(6) H(17) 102.1 .000 .000 .280 .223 .059 -.021
C(8) C(6) C(2) H(11) -79.5 .000 .000 .280 .067 .059 -.001
H(9) C(1) C(2) H(11)-162.7 .000 .000 .238 .045 .059 -.001
H(9) C(1) C(5) H(14) 18.3 .000 .000 .238 .188 .059 -.021
H(9) C(1) C(5) H(15) 138.3 .000 .000 .238 .188 .059 -.021
H(10) C(1) C(2) H(11) -41.8 .000 .000 .238 .050 .059 -.001
H(10) C(1) C(5) H(14)-102.6 .000 .000 .238 .192 .059 -.022
H(10) C(1) C(5) H(15) 17.4 .000 .000 .238 .192 .059 -.022
H(11) C(2) C(6) H(16) 41.8 .000 .000 .238 .050 .059 -.001
H(11) C(2) C(6) H(17) 162.7 .000 .000 .238 .045 .059 -.001
H(12) C(4) C(5) H(14) 132.9 .000 .000 .238 .212 .059 -.022
H(12) C(4) C(5) H(15) 12.9 .000 .000 .238 .212 .059 -.022
H(13) C(4) C(5) H(14) 9.8 .000 .000 .238 .223 .059 -.023
H(13) C(4) C(5) H(15)-110.2 .000 .000 .238 .223 .059 -.023
H(16) C(6) C(8) H(20) -17.4 .000 .000 .238 .192 .059 -.022
H(16) C(6) C(8) H(21) 102.6 .000 .000 .238 .192 .059 -.022
H(17) C(6) C(8) H(20)-138.3 .000 .000 .238 .188 .059 -.021
H(17) C(6) C(8) H(21) -18.3 .000 .000 .238 .188 .059 -.021
H(18) C(7) C(8) H(20) 110.2 .000 .000 .238 .223 .059 -.023
H(18) C(7) C(8) H(21) -9.8 .000 .000 .238 .223 .059 -.023
H(19) C(7) C(8) H(20) -12.9 .000 .000 .238 .212 .059 -.022
H(19) C(7) C(8) H(21)-132.9 .000 .000 .238 .212 .059 -.022

Molecular Shape : ASYMMETRIC ROTOR WITH KAPPA = -.620203
 Symmetry Point Group : Cs
 Symmetry Number : 1
 Chirality : no

0 FUNDAMENTAL NORMAL VIBRATIONAL FREQUENCIES
 (THEORETICALLY 57 VALUES)

Frequency : in 1/cm

A(i) : IR intensity (vs,s,m,w,vw,-- or in 10**6 cm/mole)

A(i) = -- : IR inactive

no	Frequency	Symmetry	A(i)
1.	2950.8	(A ⁺)	s
2.	2950.6	(A ⁺)	w
3.	2943.4	(A ⁺)	s
4.	2943.3	(A ⁺)	w
5.	2938.9	(A ⁺)	w
6.	2938.9	(A ⁺)	m
7.	2893.9	(A ⁺)	m
8.	2893.3	(A ⁺)	m
9.	2882.8	(A ⁺)	m
10.	2882.5	(A ⁺)	m
11.	2810.6	(A ⁺)	m
12.	2800.9	(A ⁺)	m
13.	2800.5	(A ⁺)	vw
14.	1528.7	(A ⁺)	w
15.	1482.3	(A ⁺)	w
16.	1435.4	(A ⁺)	w
17.	1422.8	(A ⁺)	w
18.	1404.7	(A ⁺)	w
19.	1402.2	(A ⁺)	w
20.	1385.8	(A ⁺)	w
21.	1379.6	(A ⁺)	w
22.	1350.7	(A ⁺)	w
23.	1334.3	(A ⁺)	w
24.	1301.4	(A ⁺)	w
25.	1295.7	(A ⁺)	w
26.	1291.4	(A ⁺)	w
27.	1276.9	(A ⁺)	m
28.	1274.6	(A ⁺)	w
29.	1204.8	(A ⁺)	w
30.	1188.5	(A ⁺)	w
31.	1168.6	(A ⁺)	w
32.	1165.1	(A ⁺)	m
33.	1147.1	(A ⁺)	vw
34.	1115.3	(A ⁺)	w
35.	1106.5	(A ⁺)	w
36.	1062.5	(A ⁺)	w
37.	1021.1	(A ⁺)	vw
38.	982.4	(A ⁺)	w
39.	980.6	(A ⁺)	vw
40.	958.3	(A ⁺)	w
41.	947.8	(A ⁺)	w
42.	942.7	(A ⁺)	--
43.	871.5	(A ⁺)	w
44.	868.1	(A ⁺)	w
45.	841.8	(A ⁺)	w
46.	796.9	(A ⁺)	w
47.	775.6	(A ⁺)	w
48.	770.3	(A ⁺)	vw
49.	631.7	(A ⁺)	w
50.	541.4	(A ⁺)	w
51.	533.6	(A ⁺)	w

52.	440.5	(A ⁺)	w
53.	342.4	(A ⁺)	w
54.	215.6	(A ⁺)	w
55.	205.2	(A ⁺)	vw
56.	132.3	(A ⁺)	vw
57.	107.9	(A ⁺)	vw
58.	(.0)	(t/r)	
59.	(.0)	(t/r)	
60.	(.0)	(t/r)	
61.	(.0)	(t/r)	
62.	(.0)	(t/r)	
63.	(.0)	(t/r)	

=====

STATISTICAL THERMODYNAMICS ANALYSIS

=====

Structure name : pyrrolizidine
 Temperature : 298.16 K
 Symmetry number : 1
 Optical isomers : 1
 Zero Point Energy : 116.170 Kcal/mol

	ENERGY (Kcal/mol)	ENTHALPY (Kcal/mol)	ENTROPY (eu)	FREE ENERGY (Kcal/mol)	HEAT CAPACITY (cal/mol/deg)
Translational	.889	1.481	40.014	-10.449	4.967
Rotational	.889	.889	27.856	-7.417	2.980
Vibrational	119.089%	119.089%	16.397*	114.200%	23.712*
Potential	42.053#	42.053#	.000	42.053#	.000
Mixing	.000	.000	.000	.000	.000
Total	162.920	163.512	84.267	138.387	31.660

Enthalpy Function (H-Ho)/T = 17.74 cal/mol/deg
 Free Energy Function -(G-Ho)/T = 66.53 cal/mol/deg

% Includes zero point energy (ZPE).
 * Excludes contribution from frequencies lower than 40 (1/cm).
 # Includes steric energy (SE).
 Internal rotation contributions are not considered

This structure has 0 imaginary frequencies,
 0 free internal rotation (fir) frequencies
 (>= 0, < 10 /cm),
 0 restricted internal rotation (rir) frequencies
 (>= 10, < 40 /cm),
 6 zero frequencies, and
 57 real frequencies.

FINAL STERIC ENERGY IS 42.0532 KCAL/MOL.

COMPRESSION 1.5977
 BENDING 15.6366
 BEND-BEND .6423
 STRETCH-BEND -.3745
 VANDERWAALS
 1,4 ENERGY 5.3839
 OTHER -.5981

TORSIONAL 20.5961
 TORSION-STRETCH -.8308
 DIPOLE-DIPOLE .0000
 CHARGE-DIPOLE .0000
 CHARGE-CHARGE .0000

COORDINATES TRANSLATED TO NEW ORIGIN WHICH IS CENTER OF MASS

C(1)	-1.34454	-1.23899	-.09466	(1)
C(2)	.00000	-.71456	.40945	(1)
N(3)	.00000	.60586	-.18942	(8)
C(4)	-1.28984	1.23513	.04343	(1)
C(5)	-2.25962	.02451	-.07102	(1)
C(6)	1.34454	-1.23899	-.09466	(1)
C(7)	1.28984	1.23513	.04343	(1)
C(8)	2.25963	.02451	-.07102	(1)
H(9)	-1.24741	-1.62094	-1.13606	(5)
H(10)	-1.73855	-2.05968	.54379	(5)
H(11)	.00000	-.62108	1.53278	(5)
H(12)	-1.32978	1.68510	1.07215	(5)
H(13)	-1.49401	2.02377	-.71276	(5)
H(14)	-2.87162	.08358	-.99893	(5)
H(15)	-2.95318	-.00206	.79937	(5)
H(16)	1.73855	-2.05968	.54379	(5)
H(17)	1.24741	-1.62094	-1.13606	(5)
H(18)	1.49401	2.02377	-.71276	(5)
H(19)	1.32978	1.68510	1.07215	(5)
H(20)	2.95318	-.00206	.79937	(5)
H(21)	2.87162	.08358	-.99893	(5)

MOMENT OF INERTIA WITH THE PRINCIPAL AXES

(1) UNIT = 10**(-39) GM*CM**2
 IX= 21.2649 IY= 45.2385 IZ= 61.4880

(2) UNIT = AU A**2
 IX= 128.0744 IY= 272.4622 IZ= 370.3299

DIPOLE MOMENT = .500 D

COMPONENTS WITH PRINCIPAL AXES

X = .0000 Y = .0307 Z = -.4987

Quinolizidine 5 (trans-conformer)CONFORMATIONAL ENERGY, PART 3: GEOMETRY AND STERIC ENERGY
OF FINAL CONFORMATION.

CONNECTED ATOMS

1- 2- 3- 4- 5- 6- 7- 10- 9-
 1- 6-
 5- 8- 9-

ATTACHED ATOMS

1- 11, 1- 12, 2- 13, 2- 14, 3- 15, 3- 16, 4- 17,
 4- 18, 5- 19, 7- 20, 7- 21, 8- 22, 8- 23, 9- 24,
 9- 25, 10- 26, 10- 27,

FINAL ATOMIC COORDINATE

ATOM	X	Y	Z	TYPE
C(1)	-1.19760	1.41015	.18163	(1)
C(2)	-2.48457	.73236	-.28964	(1)
C(3)	-2.53977	-.71066	.21300	(1)
C(4)	-1.25426	-1.44566	-.17307	(1)
C(5)	.00000	-.70024	.31069	(1)
N(6)	.00000	.66935	-.22579	(8)
C(7)	1.19760	1.41015	.18163	(1)
C(8)	1.25426	-1.44566	-.17307	(1)
C(9)	2.53977	-.71066	.21300	(1)
C(10)	2.48457	.73236	-.28964	(1)
H(11)	-1.16246	2.43881	-.24336	(5)
H(12)	-1.22129	1.52183	1.30214	(5)
H(13)	-2.52531	.74263	-1.40315	(5)
H(14)	-3.37313	1.29866	.07202	(5)
H(15)	-2.65784	-.71858	1.32117	(5)
H(16)	-3.42727	-1.23377	-.21180	(5)
H(17)	-1.21830	-1.56031	-1.28075	(5)
H(18)	-1.27151	-2.47441	.25418	(5)
H(19)	.00000	-.66311	1.43797	(5)
H(20)	1.16246	2.43881	-.24336	(5)
H(21)	1.22129	1.52183	1.30214	(5)
H(22)	1.21830	-1.56031	-1.28075	(5)
H(23)	1.27151	-2.47441	.25418	(5)
H(24)	2.65784	-.71858	1.32117	(5)
H(25)	3.42727	-1.23377	-.21180	(5)
H(26)	3.37313	1.29866	.07202	(5)
H(27)	2.52531	.74263	-1.40315	(5)

DIELECTRIC CONSTANT = 1.500

BOND LENGTHS AND STRETCHING ENERGY (28 BONDS)

ENERGY = 71.94(KS)(DR)(DR)(1-(CS)(DR)+(7/12)((CS)(DR))**2)
 DR = R-RO
 CS = 2.550

BOND	LENGTH	R(0)	K(S)	R(0)-CORR	CORR	ENERGY	E-NEG	MISCEL	KS
C(1)- C(2)	1.5290	1.5197	4.490	.0272	-.0050				
C(1)- N(6)	1.4660	1.4480	5.300	.1174					
C(1)- H(11)	1.1135	1.1111	4.710	.0020	-.0011	.0002	BH	.030	
C(1)- H(12)	1.1263	1.1235	4.304	.0024	-.0011	.0126	BH	-.376	
C(2)- C(3)	1.5290	1.5227	4.490	.0128	-.0020				
C(2)- H(13)	1.1143	1.1116	4.694	.0025	-.0004			.014	
C(2)- H(14)	1.1140	1.1116	4.694	.0020	-.0004			.014	
C(3)- C(4)	1.5303	1.5227	4.490	.0183	-.0020				
C(3)- H(15)	1.1145	1.1120	4.680	.0020					
C(3)- H(16)	1.1143	1.1120	4.680	.0018					
C(4)- C(5)	1.5372	1.5197	4.490	.0941	-.0050				
C(4)- H(17)	1.1142	1.1116	4.694	.0023	-.0004			.014	
C(4)- H(18)	1.1141	1.1116	4.694	.0021	-.0004			.014	
C(5)- N(6)	1.4709	1.4480	5.300	.1889					

S52

```

C( 5)- C( 8) 1.5372 1.5197 4.490 .0941 -.0050
C( 5)- H( 19) 1.1279 1.1235 4.434 .0060 -.0011 .0126 BH -.376
N( 6)- C( 7) 1.4660 1.4480 5.300 .1174
C( 7)- C( 10) 1.5290 1.5197 4.490 .0272 -.0050
C( 7)- H( 20) 1.1135 1.1111 4.710 .0020 -.0011 .0002 BH .030
C( 7)- H( 21) 1.1263 1.1235 4.304 .0024 -.0011 .0126 BH -.376
C( 8)- C( 9) 1.5303 1.5227 4.490 .0183 -.0020
C( 8)- H( 22) 1.1142 1.1116 4.694 .0023 -.0004 .014
C( 8)- H( 23) 1.1141 1.1116 4.694 .0021 -.0004 .014
C( 9)- C( 10) 1.5290 1.5227 4.490 .0128 -.0020
C( 9)- H( 24) 1.1145 1.1120 4.680 .0020
C( 9)- H( 25) 1.1143 1.1120 4.680 .0018
C( 10)- H( 26) 1.1140 1.1116 4.694 .0020 -.0004 .014
C( 10)- H( 27) 1.1143 1.1116 4.694 .0025 -.0004 .014

```

NON-BONDED DISTANCES, VDW AND EPR ENERGY (266 PAIRS)

```

E(VDW) = KV*(1.84(10**5)EXP(-12.00/P) - 2.25(P**6))
E(EPR) = C*KV*(1.84(10**5)EXP(-12.00/Q) - 2.25(Q**6))
E(HBD) = EP1-EP2*COS(THETA)*RTH/RTH0
          EP1 = KHB*1.84(10**5)*EXP(-12.0/P)
          EP2 = KHB*2.25(P**6)

```

IF P > 3.020, THEN,

```

E(VDW) = KV(192.270)(P**2)
E(HBD) = EP1-EP2*COS(THETA)*RTH/RTH0
          EP1 = KHB*(192.270*P**2+1706.96)
          EP2 = KHB*1706.96

```

WHERE RV = RVDW(I) + RVDW(K)

KV = SQRT(EPS(I)*EPS(K))

KHB = EPS/DIELEC FOR HYDROGEN BOND

P = (RV/R) OR (RV/R#)

C = SCALE FACTOR

Q = RV/R, WHERE R IS MODIFIED DISTANCE

THETA = ANGLE H-X-Y IN HYDROGEN BOND X-H...Y

RTH = BOND LENGTH X-H IN X-H...Y

RTH0 = NATURAL BOND LENGTH X-H

IN THE VDW CALCULATIONS THE HYDROGEN ATOMS ARE RELOCATED
SO THAT THE ATTACHED HYDROGEN DISTANCE IS REDUCED BY .923

IN THE VDW CALCULATIONS THE DEUTERIUM ATOMS ARE RELOCATED
SO THAT THE ATTACHED DEUTERIUM DISTANCE IS REDUCED BY .923

** INTERACTIONS OF LESS THAN 0.1 KCAL/MOL ARE NOT PRINTED **

ATOM PAIR	R	R#	RV	KV	ENERGY
C(1), C(4)	2.8783		4.080	.0270	.5534 1,4
C(1), H(15)	2.8218	2.7832	3.560	.0230	.1300 1,4
C(1), H(19)	2.7039	2.6669	3.560	.0230	.2350 1,4
C(1), H(20)	2.6093	2.5764	3.560	.0230	.3558 1,4
C(1), H(21)	2.6682	2.6311	3.560	.0230	.2780 1,4
C(2), C(5)	2.9302		4.080	.0270	.4555 1,4
C(2), H(17)	2.8004	2.7628	3.560	.0230	.1451 1,4
C(3), N(6)	2.9236		3.970	.0341	.4300 1,4
C(3), H(12)	2.8122	2.7739	3.560	.0230	.1367 1,4
C(3), H(19)	2.8202	2.7835	3.560	.0230	.1297 1,4
C(4), H(13)	2.8138	2.7753	3.560	.0230	.1357 1,4
C(4), H(22)	2.7118	2.6802	3.560	.0230	.2204 1,4
C(4), H(23)	2.7605	2.7258	3.560	.0230	.1759 1,4
C(5), C(10)	2.9302		4.080	.0270	.4555 1,4
C(5), H(12)	2.7225	2.6844	3.560	.0230	.2160 1,4
C(5), H(15)	2.8435	2.8057	3.560	.0230	.1146 1,4
C(5), H(21)	2.7225	2.6844	3.560	.0230	.2160 1,4
C(5), H(24)	2.8435	2.8057	3.560	.0230	.1146 1,4
N(6), C(9)	2.9236		3.970	.0341	.4300 1,4
N(6), H(13)	2.7872	2.7492	3.550	.0293	.1908 1,4
N(6), H(17)	2.7511	2.7136	3.550	.0293	.2296 1,4
N(6), H(22)	2.7511	2.7136	3.550	.0293	.2296 1,4

S53

N(6), H(27)	2.7872	2.7492	3.550	.0293	.1908	1,4
C(7), C(8)	2.8783	4.080	.0270	.5534	1,4	
C(7), H(11)	2.6093	2.5764	3.560	.0230	.3558	1,4
C(7), H(12)	2.6682	2.6311	3.560	.0230	.2780	1,4
C(7), H(19)	2.7039	2.6669	3.560	.0230	.2350	1,4
C(7), H(24)	2.8218	2.7832	3.560	.0230	.1300	1,4
C(8), H(17)	2.7118	2.6802	3.560	.0230	.2204	1,4
C(8), H(18)	2.7605	2.7258	3.560	.0230	.1759	1,4
C(8), H(27)	2.8138	2.7753	3.560	.0230	.1357	1,4
C(9), H(19)	2.8202	2.7835	3.560	.0230	.1297	1,4
C(9), H(21)	2.8122	2.7739	3.560	.0230	.1367	1,4
C(10), H(22)	2.8004	2.7628	3.560	.0230	.1451	1,4
H(11), H(13)	2.4657	2.3840	3.240	.0200	.2549	1,4
H(11), H(14)	2.5073	2.4213	3.240	.0200	.2107	1,4
H(11), H(20)	2.3249	2.3303	3.240	.0200	.3318	
H(12), H(14)	2.4887	2.4058	3.240	.0200	.2283	1,4
H(12), H(19)	2.5068	2.5009	3.240	.0200	.1365	
H(12), H(21)	2.4426	2.4389	3.240	.0200	.1920	
H(13), H(16)	2.4777	2.3961	3.240	.0200	.2398	1,4
H(14), H(15)	2.4782	2.3965	3.240	.0200	.2393	1,4
H(14), H(16)	2.5489	2.4593	3.240	.0200	.1722	1,4
H(15), H(18)	2.4786	2.3964	3.240	.0200	.2394	1,4
H(16), H(17)	2.4756	2.3941	3.240	.0200	.2423	1,4
H(16), H(18)	2.5305	2.4428	3.240	.0200	.1881	1,4
H(17), H(22)	2.4366	2.4421	3.240	.0200	.1888	
H(18), H(19)	2.5098	2.4249	3.240	.0200	.2067	1,4
H(18), H(23)	2.5430	2.5404	3.240	.0200	.1081	
H(19), H(21)	2.5068	2.5009	3.240	.0200	.1365	
H(19), H(23)	2.5098	2.4249	3.240	.0200	.2067	1,4
H(20), H(26)	2.5073	2.4213	3.240	.0200	.2107	1,4
H(20), H(27)	2.4657	2.3840	3.240	.0200	.2549	1,4
H(21), H(26)	2.4887	2.4058	3.240	.0200	.2283	1,4
H(22), H(25)	2.4756	2.3941	3.240	.0200	.2423	1,4
H(23), H(24)	2.4786	2.3964	3.240	.0200	.2394	1,4
H(23), H(25)	2.5305	2.4428	3.240	.0200	.1881	1,4
H(24), H(26)	2.4782	2.3965	3.240	.0200	.2393	1,4
H(25), H(26)	2.5489	2.4593	3.240	.0200	.1722	1,4
H(25), H(27)	2.4777	2.3961	3.240	.0200	.2398	1,4

BOND ANGLES, BENDING AND STRETCH-BEND ENERGIES (57 ANGLES)

$$EB = 0.021914(KB)(DT)(DT)(1+CF*DT+QF*DT**2+PF*DT**3+SF*DT**4)$$

$$DT = THETA-TZERO$$

$$CF = -1400.000E-5$$

$$QF = 5.600E-5$$

$$PF = -.070E-5$$

$$SF = .022E-6$$

$$ESB(J) = 2.51124(KSB(J))(DT)(DR1+DR2)$$

$$DR(I) = R(I) - R0(I)$$

$$EBDBD = -0.02191418(KBB1)(DT1)(KBB2)(DT2)$$

A T O M S		THETA	TZERO	KB	EB	KSB	ESB
C(2)- C(1)- N(6)	112.207	111.000	.780	.0245	.13	.0107	
C(2)- C(1)- H(11)	108.567	109.310	.590	.0072	.08	-.0018	
C(2)- C(1)- H(12)	109.444	109.310	.590	.0002	.08	.0003	
N(6)- C(1)- H(11)	109.571	109.300	.820	.0013	.08	.0011	
N(6)- C(1)- H(12)	110.107	109.300	.820	.0116	.08	.0034	
H(11)- C(1)- H(12)	106.784	107.600	.550	.0081			
C(1)- C(2)- C(3)	110.329	111.000	.670	.0067	.13	-.0034	
C(1)- C(2)- H(13)	109.554	109.310	.590	.0008	.08	.0006	
C(1)- C(2)- H(14)	110.241	109.310	.590	.0111	.08	.0022	
C(3)- C(2)- H(13)	109.625	109.310	.590	.0013	.08	.0006	
C(3)- C(2)- H(14)	110.134	109.310	.590	.0087	.08	.0015	
H(13)- C(2)- H(14)	106.892	107.600	.550	.0061			
C(2)- C(3)- C(4)	109.878	111.000	.670	.0188	.13	-.0051	
C(2)- C(3)- H(15)	109.719	109.310	.590	.0021	.08	.0007	
C(2)- C(3)- H(16)	110.271	109.310	.590	.0118	.08	.0017	
C(4)- C(3)- H(15)	109.660	109.310	.590	.0016	.08	.0007	
C(4)- C(3)- H(16)	110.328	109.310	.590	.0132	.08	.0020	
H(15)- C(3)- H(16)	106.938	107.600	.550	.0053			

S54

C(3)-C(4)-C(5)	111.909	111.000	.670	.0120	.13	.0074
C(3)-C(4)-H(17)	109.107	109.310	.590	.0005	.08	-.0004
C(3)-C(4)-H(18)	109.497	109.310	.590	.0004	.08	.0004
C(5)-C(4)-H(17)	109.661	109.310	.590	.0016	.08	.0014
C(5)-C(4)-H(18)	109.861	109.310	.590	.0039	.08	.0022
H(17)-C(4)-H(18)	106.664	107.600	.550	.0107		
C(4)-C(5)-N(6)	109.679	108.000	.780	.0471	.13	.0221
C(4)-C(5)-C(8)	109.365	110.200	.670	.0104	.13	-.0095
C(4)-C(5)-H(19)	109.300	109.800	.590	.0033	.08	-.0022
N(6)-C(5)-C(8)	109.679	108.000	.780	.0471	.13	.0221
N(6)-C(5)-H(19)	109.504	109.300	.820	.0007	.08	.0011
C(8)-C(5)-H(19)	109.300	109.800	.590	.0033	.08	-.0022
C(1)-N(6)-C(5)	111.664	107.200	.720	.2951	.05	.0229
C(1)-N(6)-C(7)	109.560	107.200	.720	.0850	.05	.0106
C(5)-N(6)-C(7)	111.664	107.200	.720	.2951	.05	.0229
N(6)-C(7)-C(10)	112.207	111.000	.780	.0245	.13	.0107
N(6)-C(7)-H(20)	109.571	109.300	.820	.0013	.08	.0011
N(6)-C(7)-H(21)	110.107	109.300	.820	.0116	.08	.0034
C(10)-C(7)-H(20)	108.567	109.310	.590	.0072	.08	-.0018
C(10)-C(7)-H(21)	109.444	109.310	.590	.0002	.08	.0003
H(20)-C(7)-H(21)	106.784	107.600	.550	.0081		
C(5)-C(8)-C(9)	111.909	111.000	.670	.0120	.13	.0074
C(5)-C(8)-H(22)	109.661	109.310	.590	.0016	.08	.0014
C(5)-C(8)-H(23)	109.861	109.310	.590	.0039	.08	.0022
C(9)-C(8)-H(22)	109.107	109.310	.590	.0005	.08	-.0004
C(9)-C(8)-H(23)	109.497	109.310	.590	.0004	.08	.0004
H(22)-C(8)-H(23)	106.664	107.600	.550	.0107		
C(8)-C(9)-C(10)	109.878	111.000	.670	.0188	.13	-.0051
C(8)-C(9)-H(24)	109.660	109.310	.590	.0016	.08	.0007
C(8)-C(9)-H(25)	110.328	109.310	.590	.0132	.08	.0020
C(10)-C(9)-H(24)	109.719	109.310	.590	.0021	.08	.0007
C(10)-C(9)-H(25)	110.271	109.310	.590	.0118	.08	.0017
H(24)-C(9)-H(25)	106.938	107.600	.550	.0053		
C(7)-C(10)-C(9)	110.329	111.000	.670	.0067	.13	-.0034
C(7)-C(10)-H(26)	110.241	109.310	.590	.0111	.08	.0022
C(7)-C(10)-H(27)	109.554	109.310	.590	.0008	.08	.0006
C(9)-C(10)-H(26)	110.134	109.310	.590	.0087	.08	.0015
C(9)-C(10)-H(27)	109.625	109.310	.590	.0013	.08	.0006
H(26)-C(10)-H(27)	106.892	107.600	.550	.0061		

DIHEDRAL ANGLES, TORSIONAL ENERGY (ET) (90 ANGLES)

$$ET = (V1/2)(1+\cos(W)) + (V2/2)(1-\cos(2W)) + (V3/2)(1+\cos(3W))$$

$$ETS = -11.995 \cdot (R-R0) \cdot ((KTS1/2)(1+\cos(W)) + (KTS2/2)(1-\cos(2W)) + (KTS3/2)(1+\cos(3W)))$$

SIGN OF ANGLE A-B-C-D : WHEN LOOKING THROUGH B TOWARD C,
IF D IS COUNTERCLOCKWISE FROM A, NEGATIVE.

A T O M S		OMEGA	V1	V2	V3	ET	KTS3	ETS
C(1) C(2) C(3) C(4)	-52.7	.185	.170	.520	.275	.059	.000	
C(1) C(2) C(3) H(15)	68.0	.000	.000	.280	.012	.059	.000	
C(1) C(2) C(3) H(16)	-174.5	.000	.000	.280	.006	.059	.000	
C(1) N(6) C(5) C(4)	58.4	.958	-.155	.766	.619	.061	.000	
C(1) N(6) C(5) C(8)	178.5	.958	-.155	.766	.001	.061	.000	
C(1) N(6) C(5) H(19)	-61.5	.072	-.012	.563	.045	.061	.000	
C(1) N(6) C(7) C(10)	-176.5	.958	-.155	.766	.007	.061	.000	
C(1) N(6) C(7) H(20)	-55.8	.072	-.012	.563	.055	.061	.000	
C(1) N(6) C(7) H(21)	61.3	.072	-.012	.563	.045	.061	.000	
C(2) C(1) N(6) C(5)	-59.3	.958	-.155	.766	.610	.061	.000	
C(2) C(1) N(6) C(7)	176.5	.958	-.155	.766	.007	.061	.000	
C(2) C(3) C(4) C(5)	54.2	.185	.170	.520	.270	.059	.000	
C(2) C(3) C(4) H(17)	-67.4	.000	.000	.280	.010	.059	.000	
C(2) C(3) C(4) H(18)	176.3	.000	.000	.280	.003	.059	.000	
C(3) C(2) C(1) N(6)	55.8	-.302	.696	.499	.247	.059	.000	
C(3) C(2) C(1) H(11)	177.1	.000	.000	.280	.002	.059	.000	
C(3) C(2) C(1) H(12)	-66.7	.000	.000	.280	.009	.059	.000	
C(3) C(4) C(5) N(6)	-56.6	-.302	.696	.499	.255	.059	.000	

C(3) C(4) C(5) C(8)-176.9	.185	.170	.520	.004	.059	.000
C(3) C(4) C(5) H(19) 63.5	.000	.000	.280	.002	.059	.000
C(4) C(3) C(2) H(13) 68.0	.000	.000	.280	.012	.059	.000
C(4) C(3) C(2) H(14)-174.6	.000	.000	.280	.006	.059	.000
C(4) C(5) N(6) C(7)-178.5	.958	-.155	.766	.001	.061	.000
C(4) C(5) C(8) C(9) 176.9	.185	.170	.520	.004	.059	.000
C(4) C(5) C(8) H(22) 55.7	.000	.000	.280	.004	.059	.000
C(4) C(5) C(8) H(23) -61.2	.000	.000	.280	.000	.059	.000
C(5) C(4) C(3) H(15) -66.5	.000	.000	.280	.008	.059	.000
C(5) C(4) C(3) H(16) 176.0	.000	.000	.280	.003	.059	.000
C(5) N(6) C(1) H(11)-179.9	.072	-.012	.563	.000	.061	.000
C(5) N(6) C(1) H(12) 62.9	.072	-.012	.563	.046	.061	.000
C(5) N(6) C(7) C(10) 59.3	.958	-.155	.766	.610	.061	.000
C(5) N(6) C(7) H(20) 179.9	.072	-.012	.563	.000	.061	.000
C(5) N(6) C(7) H(21) -62.9	.072	-.012	.563	.046	.061	.000
C(5) C(8) C(9) C(10) -54.2	.185	.170	.520	.270	.059	.000
C(5) C(8) C(9) H(24) 66.5	.000	.000	.280	.008	.059	.000
C(5) C(8) C(9) H(25)-176.0	.000	.000	.280	.003	.059	.000
N(6) C(1) C(2) H(13) -64.9	.000	.000	.374	.006	.059	.000
N(6) C(1) C(2) H(14) 177.7	.000	.000	.374	.001	.059	.000
N(6) C(5) C(4) H(17) 64.6	.000	.000	.374	.005	.059	.000
N(6) C(5) C(4) H(18)-178.5	.000	.000	.374	.001	.059	.000
N(6) C(5) C(8) C(9) 56.6	-.302	.696	.499	.255	.059	.000
N(6) C(5) C(8) H(22) -64.6	.000	.000	.374	.005	.059	.000
N(6) C(5) C(8) H(23) 178.5	.000	.000	.374	.001	.059	.000
N(6) C(7) C(10) C(9) -55.8	-.302	.696	.499	.247	.059	.000
N(6) C(7) C(10) H(26)-177.7	.000	.000	.374	.001	.059	.000
N(6) C(7) C(10) H(27) 64.9	.000	.000	.374	.006	.059	.000
C(7) N(6) C(1) H(11) 55.8	.072	-.012	.563	.055	.061	.000
C(7) N(6) C(1) H(12) -61.3	.072	-.012	.563	.045	.061	.000
C(7) N(6) C(5) C(8) -58.4	.958	-.155	.766	.619	.061	.000
C(7) N(6) C(5) H(19) 61.5	.072	-.012	.563	.045	.061	.000
C(7) C(10) C(9) C(8) 52.7	.185	.170	.520	.275	.059	.000
C(7) C(10) C(9) H(24) -68.0	.000	.000	.280	.012	.059	.000
C(7) C(10) C(9) H(25) 174.5	.000	.000	.280	.006	.059	.000
C(8) C(5) C(4) H(17) -55.7	.000	.000	.280	.004	.059	.000
C(8) C(5) C(4) H(18) 61.2	.000	.000	.280	.000	.059	.000
C(8) C(9) C(10) H(26) 174.6	.000	.000	.280	.006	.059	.000
C(8) C(9) C(10) H(27) -68.0	.000	.000	.280	.012	.059	.000
C(9) C(8) C(5) H(19) -63.5	.000	.000	.280	.002	.059	.000
C(9) C(10) C(7) H(20)-177.1	.000	.000	.280	.002	.059	.000
C(9) C(10) C(7) H(21) 66.7	.000	.000	.280	.009	.059	.000
C(10) C(9) C(8) H(22) 67.4	.000	.000	.280	.010	.059	.000
C(10) C(9) C(8) H(23)-176.3	.000	.000	.280	.003	.059	.000
H(11) C(1) C(2) H(13) 56.3	.000	.000	.238	.002	.059	.000
H(11) C(1) C(2) H(14) -61.0	.000	.000	.238	.000	.059	.000
H(12) C(1) C(2) H(13) 172.5	.000	.000	.238	.009	.059	.000
H(12) C(1) C(2) H(14) 55.2	.000	.000	.238	.004	.059	.000
H(13) C(2) C(3) H(15)-171.3	.000	.000	.238	.012	.059	.000
H(13) C(2) C(3) H(16) -53.8	.000	.000	.238	.006	.059	.000
H(14) C(2) C(3) H(15) -54.0	.000	.000	.238	.006	.059	.000
H(14) C(2) C(3) H(16) 63.6	.000	.000	.238	.002	.059	.000
H(15) C(3) C(4) H(17) 172.0	.000	.000	.238	.010	.059	.000
H(15) C(3) C(4) H(18) 55.6	.000	.000	.238	.003	.059	.000
H(16) C(3) C(4) H(17) 54.4	.000	.000	.238	.005	.059	.000
H(16) C(3) C(4) H(18) -62.0	.000	.000	.238	.001	.059	.000
H(17) C(4) C(5) H(19)-175.3	.000	.000	.238	.004	.059	.000
H(18) C(4) C(5) H(19) -58.4	.000	.000	.238	.000	.059	.000
H(19) C(5) C(8) H(22) 175.3	.000	.000	.238	.004	.059	.000
H(19) C(5) C(8) H(23) 58.4	.000	.000	.238	.000	.059	.000
H(20) C(7) C(10) H(26) 61.0	.000	.000	.238	.000	.059	.000
H(20) C(7) C(10) H(27) -56.3	.000	.000	.238	.002	.059	.000
H(21) C(7) C(10) H(26) -55.2	.000	.000	.238	.004	.059	.000
H(21) C(7) C(10) H(27)-172.5	.000	.000	.238	.009	.059	.000
H(22) C(8) C(9) H(24)-172.0	.000	.000	.238	.010	.059	.000
H(22) C(8) C(9) H(25) -54.4	.000	.000	.238	.005	.059	.000
H(23) C(8) C(9) H(24) -55.6	.000	.000	.238	.003	.059	.000
H(23) C(8) C(9) H(25) 62.0	.000	.000	.238	.001	.059	.000
H(24) C(9) C(10) H(26) 54.0	.000	.000	.238	.006	.059	.000
H(24) C(9) C(10) H(27) 171.3	.000	.000	.238	.012	.059	.000
H(25) C(9) C(10) H(26) -63.6	.000	.000	.238	.002	.059	.000

S56

H(25) C(9) C(10) H(27) 53.8 .000 .000 .238 .006 .059 .000

=====

NORMAL MODE VIBRATIONAL ANALYSIS

=====

Molecular Shape : ASYMMETRIC ROTOR WITH KAPPA = -.705886

Symmetry Point Group : Cs

Symmetry Number : 1

Chirality : no

0 FUNDAMENTAL NORMAL VIBRATIONAL FREQUENCIES
(THEORETICALLY 75 VALUES)

Frequency : in 1/cm

A(i) : IR intensity (vs,s,m,w,vw,-- or in 10**6 cm/mole)

A(i) = -- : IR inactive

no	Frequency	Symmetry	A(i)
1.	2932.3	(A ⁺)	vs
2.	2932.0	(A ⁺)	w
3.	2929.8	(A ⁺)	m
4.	2929.2	(A ⁺)	w
5.	2927.7	(A ⁺)	m
6.	2927.5	(A ⁺)	m
7.	2915.5	(A ⁺)	s
8.	2913.0	(A ⁺)	vw
9.	2886.0	(A ⁺)	m
10.	2885.4	(A ⁺)	m
11.	2878.9	(A ⁺)	m
12.	2877.8	(A ⁺)	w
13.	2869.2	(A ⁺)	m
14.	2868.7	(A ⁺)	w
15.	2800.9	(A ⁺)	m
16.	2774.0	(A ⁺)	m
17.	2772.0	(A ⁺)	vw
18.	1585.6	(A ⁺)	w
19.	1551.7	(A ⁺)	w
20.	1496.1	(A ⁺)	w
21.	1496.1	(A ⁺)	vw
22.	1468.9	(A ⁺)	w
23.	1464.8	(A ⁺)	vw
24.	1464.6	(A ⁺)	--
25.	1462.8	(A ⁺)	w
26.	1457.7	(A ⁺)	w
27.	1453.9	(A ⁺)	w
28.	1437.6	(A ⁺)	w
29.	1430.3	(A ⁺)	w
30.	1421.5	(A ⁺)	w
31.	1406.3	(A ⁺)	w
32.	1403.0	(A ⁺)	m
33.	1386.1	(A ⁺)	w
34.	1360.3	(A ⁺)	w
35.	1352.7	(A ⁺)	m
36.	1309.2	(A ⁺)	vw
37.	1304.6	(A ⁺)	w
38.	1263.7	(A ⁺)	w
39.	1221.8	(A ⁺)	w
40.	1219.1	(A ⁺)	w
41.	1208.7	(A ⁺)	w
42.	1206.0	(A ⁺)	vw
43.	1197.5	(A ⁺)	w
44.	1157.0	(A ⁺)	w
45.	1125.2	(A ⁺)	w
46.	1086.0	(A ⁺)	w

47.	1062.5	(A`)	w
48.	1053.4	(A")	vw
49.	1042.2	(A`)	w
50.	1017.4	(A")	w
51.	996.6	(A")	w
52.	965.0	(A`)	w
53.	952.0	(A`)	w
54.	949.5	(A")	w
55.	901.5	(A`)	w
56.	899.4	(A")	w
57.	857.4	(A`)	w
58.	847.8	(A")	vw
59.	837.5	(A")	w
60.	816.7	(A")	vw
61.	814.0	(A`)	w
62.	754.7	(A`)	w
63.	586.5	(A")	w
64.	530.5	(A`)	w
65.	467.1	(A`)	w
66.	465.7	(A")	w
67.	382.6	(A")	w
68.	371.9	(A`)	w
69.	346.3	(A`)	w
70.	342.1	(A")	vw
71.	297.7	(A`)	w
72.	289.4	(A`)	w
73.	224.7	(A")	vw
74.	142.9	(A`)	w
75.	129.5	(A")	vw
76.	(.0)	(t/r)	
77.	(.0)	(t/r)	
78.	(.0)	(t/r)	
79.	(.0)	(t/r)	
80.	(.0)	(t/r)	
81.	(.0)	(t/r)	

=====

STATISTICAL THERMODYNAMICS ANALYSIS

=====

Structure name : MMX chinolys
Temperature : 298.16 K
Symmetry number : 1
Optical isomers : 1
Zero Point Energy : 154.053 Kcal/mol

	ENERGY	ENTHALPY	ENTROPY	FREE ENERGY	HEAT CAPACITY
	(Kcal/mol)	(Kcal/mol)	(eu)	(Kcal/mol)	(cal/mol/deg)
Translational	.889	1.481	40.684	-10.649	4.967
Rotational	.889	.889	29.416	-7.882	2.980
Vibrational	157.893%	157.893%	20.484*	151.785%	31.656*
Potential	18.978#	18.978#	.000	18.978#	.000
Mixing	.000	.000	.000	.000	.000
Total	178.649	179.241	90.585	152.232	39.604

Enthalpy Function (H-Ho)/T = 20.83 cal/mol/deg
Free Energy Function -(G-Ho)/T = 69.76 cal/mol/deg

% Includes zero point energy (ZPE).
* Excludes contribution from frequencies lower than 40 (1/cm).
Includes steric energy (SE).
Internal rotation contributions are not considered

This structure has 0 imaginary frequencies,
0 free internal rotation (fir) frequencies
(>= 0, < 10 /cm),
0 restricted internal rotation (rir) frequencies
(>= 10, < 40 /cm),
6 zero frequencies, and

75 real frequencies.

FINAL STERIC ENERGY IS 18.9785 KCAL/MOL.

```

COMPRESSION      .7691
BENDING          1.1258
BEND-BEND        -.0544
STRETCH-BEND     .1404
VANDERWAALS
  1,4 ENERGY    12.0720
  OTHER          -.3287

TORSIONAL        5.2631
TORSION-STRETCH -.0088
DIPOLE-DIPOLE    .0000
CHARGE-DIPOLE    .0000
CHARGE-CHARGE    .0000

```

COORDINATES TRANSLATED TO NEW ORIGIN WHICH IS CENTER OF MASS

```

C( 1) -1.19760  1.41015  .18163 ( 1)
C( 2) -2.48457  .73236  -.28964 ( 1)
C( 3) -2.53977  -.71066  .21300 ( 1)
C( 4) -1.25426  -1.44566  -.17307 ( 1)
C( 5)  .00000  -.70024  .31069 ( 1)
N( 6)  .00000  .66935  -.22579 ( 8)
C( 7)  1.19760  1.41015  .18163 ( 1)
C( 8)  1.25426  -1.44566  -.17307 ( 1)
C( 9)  2.53977  -.71066  .21300 ( 1)
C(10)  2.48457  .73236  -.28964 ( 1)
H(11) -1.16246  2.43881  -.24336 ( 5)
H(12) -1.22129  1.52183  1.30214 ( 5)
H(13) -2.52531  .74263  -1.40315 ( 5)
H(14) -3.37313  1.29866  .07202 ( 5)
H(15) -2.65784  -.71858  1.32117 ( 5)
H(16) -3.42727  -1.23377  -.21180 ( 5)
H(17) -1.21830  -1.56031  -1.28075 ( 5)
H(18) -1.27151  -2.47441  .25418 ( 5)
H(19)  .00000  -.66311  1.43797 ( 5)
H(20)  1.16246  2.43881  -.24336 ( 5)
H(21)  1.22129  1.52183  1.30214 ( 5)
H(22)  1.21830  -1.56031  -1.28075 ( 5)
H(23)  1.27151  -2.47441  .25418 ( 5)
H(24)  2.65784  -.71858  1.32117 ( 5)
H(25)  3.42727  -1.23377  -.21180 ( 5)
H(26)  3.37313  1.29866  .07202 ( 5)
H(27)  2.52531  .74263  -1.40315 ( 5)

```

MOMENT OF INERTIA WITH THE PRINCIPAL AXES

(1) UNIT = 10**(-39) GM*CM**2
 IX= 33.3970 IY= 80.3570 IZ= 106.0721

(2) UNIT = AU A**2
 IX= 201.1432 IY= 483.9740 IZ= 638.8511

DIPOLE MOMENT = .628 D

COMPONENTS WITH PRINCIPAL AXES

X = .0000 Y = -.0541 Z = -.6260

Compound 5 (cis-conformer)CONFORMATIONAL ENERGY, PART 3: GEOMETRY AND STERIC ENERGY
OF FINAL CONFORMATION.

CONNECTED ATOMS

1- 2- 3- 4- 5- 6- 7- 10- 9-
 1- 6-
 5- 8- 9-

ATTACHED ATOMS

1- 11, 1- 12, 2- 13, 2- 14, 3- 15, 3- 16, 4- 17,
 4- 18, 5- 19, 7- 20, 7- 21, 8- 22, 8- 23, 9- 24,
 9- 25, 10- 26, 10- 27,

FINAL ATOMIC COORDINATE

ATOM	X	Y	Z	TYPE
C(1)	.68532	1.35073	.45088	(1)
C(2)	2.17026	.98612	.42379	(1)
C(3)	2.35209	-.53314	.43216	(1)
C(4)	1.53276	-1.17101	-.69411	(1)
C(5)	.05374	-.75523	-.67458	(1)
N(6)	-.05076	.70884	-.64019	(8)
C(7)	-1.44542	1.14516	-.72454	(1)
C(8)	-.73292	-1.38666	.48506	(1)
C(9)	-2.20371	-.95250	.45485	(1)
C(10)	-2.32372	.57417	.39404	(1)
H(11)	.24836	1.06751	1.44663	(5)
H(12)	.58745	2.45634	.36406	(5)
H(13)	2.64075	1.41197	-.49223	(5)
H(14)	2.69378	1.43984	1.29620	(5)
H(15)	3.43018	-.78940	.31323	(5)
H(16)	2.03384	-.94595	1.41625	(5)
H(17)	1.97781	-.87346	-1.67207	(5)
H(18)	1.61519	-2.28044	-.63963	(5)
H(19)	-.40428	-1.11071	-1.62849	(5)
H(20)	-1.49457	2.25684	-.71765	(5)
H(21)	-1.86111	.83040	-1.70808	(5)
H(22)	-.67431	-2.49716	.41777	(5)
H(23)	-.28505	-1.10984	1.46434	(5)
H(24)	-2.70166	-1.39770	-.43760	(5)
H(25)	-2.73940	-1.34466	1.34986	(5)
H(26)	-2.02779	1.01245	1.37367	(5)
H(27)	-3.38655	.86456	.22859	(5)

DIELECTRIC CONSTANT = 1.500

BOND LENGTHS AND STRETCHING ENERGY (28 BONDS)

ENERGY = 71.94(KS)(DR)(DR)(1-(CS)(DR)+(7/12)((CS)(DR))**2)
 DR = R-RO
 CS = 2.550

BOND	LENGTH	R(0)	K(S)	R(0)-CORR	CORR	ENERGY	E-NEG	MISCEL	KS
C(1)- C(2)	1.5293	1.5197	4.490	.0290	-.0050				
C(1)- N(6)	1.4643	1.4480	5.300	.0976					
C(1)- H(11)	1.1237	1.1235	4.304	.0000	-.0011	.0126	BH	-.376	
C(1)- H(12)	1.1133	1.1111	4.710	.0017	-.0011	.0002	BH	.030	
C(2)- C(3)	1.5301	1.5227	4.490	.0175	-.0020				
C(2)- H(13)	1.1144	1.1116	4.694	.0026	-.0004			.014	
C(2)- H(14)	1.1140	1.1116	4.694	.0020	-.0004			.014	
C(3)- C(4)	1.5319	1.5227	4.490	.0266	-.0020				
C(3)- H(15)	1.1145	1.1120	4.680	.0021					
C(3)- H(16)	1.1136	1.1120	4.680	.0009					
C(4)- C(5)	1.5365	1.5197	4.490	.0872	-.0050				
C(4)- H(17)	1.1149	1.1116	4.694	.0037	-.0004			.014	
C(4)- H(18)	1.1138	1.1116	4.694	.0017	-.0004			.014	
C(5)- N(6)	1.4682	1.4480	5.300	.1477					

S60

```

C( 5)- C( 8) 1.5370 1.5197 4.490 .0922 -.0050
C( 5)- H( 19) 1.1163 1.1109 4.844 .0098 -.0011 .0000 BH .034
N( 6)- C( 7) 1.4638 1.4480 5.300 .0909
C( 7)- C( 10) 1.5325 1.5197 4.490 .0515 -.0050
C( 7)- H( 20) 1.1128 1.1111 4.709 .0009 -.0011 .0002 BH .029
C( 7)- H( 21) 1.1132 1.1109 4.716 .0018 -.0011 .0000 BH .036
C( 8)- C( 9) 1.5338 1.5227 4.490 .0389 -.0020
C( 8)- H( 22) 1.1141 1.1116 4.694 .0021 -.0004 .014
C( 8)- H( 23) 1.1118 1.1116 4.694 .0000 -.0004 .014
C( 9)- C( 10) 1.5326 1.5227 4.490 .0308 -.0020
C( 9)- H( 24) 1.1147 1.1120 4.680 .0025
C( 9)- H( 25) 1.1144 1.1120 4.680 .0019
C( 10)- H( 26) 1.1133 1.1116 4.694 .0010 -.0004 .014
C( 10)- H( 27) 1.1141 1.1116 4.694 .0022 -.0004 .014

```

NON-BONDED DISTANCES, VDW AND EPR ENERGY (266 PAIRS)

```

E(VDW) = KV*(1.84(10**5)EXP(-12.00/P) - 2.25(P**6))
E(EPR) = C*KV*(1.84(10**5)EXP(-12.00/Q) - 2.25(Q**6))
E(HBD) = EP1-EP2*COS(THETA)*RTH/RTH0
EP1 = KHB*1.84(10**5)*EXP(-12.0/P)
EP2 = KHB*2.25(P**6)

```

IF P > 3.020, THEN,

```

E(VDW) = KV(192.270)/(P**2)
E(HBD) = EP1-EP2*COS(THETA)*RTH/RTH0
EP1 = KHB*(192.270*P**2+1706.96)
EP2 = KHB*1706.96

```

WHERE RV = RVDW(I) + RVDW(K)

KV = SQRT(EPS(I)*EPS(K))

KHB = EPS/DIELEC FOR HYDROGEN BOND

P = (RV/R) OR (RV/R#)

C = SCALE FACTOR

Q = RV/R, WHERE R IS MODIFIED DISTANCE

THETA = ANGLE H-X-Y IN HYDROGEN BOND X-H...Y

RTH = BOND LENGTH X-H IN X-H...Y

RTH0 = NATURAL BOND LENGTH X-H

IN THE VDW CALCULATIONS THE HYDROGEN ATOMS ARE RELOCATED
SO THAT THE ATTACHED HYDROGEN DISTANCE IS REDUCED BY .923

IN THE VDW CALCULATIONS THE DEUTERIUM ATOMS ARE RELOCATED
SO THAT THE ATTACHED DEUTERIUM DISTANCE IS REDUCED BY .923

** INTERACTIONS OF LESS THAN 0.1 KCAL/MOL ARE NOT PRINTED **

ATOM PAIR	R	R#	RV	KV	ENERGY
C(1), C(4)	2.8963		4.080	.0270	.5176 1,4
C(1), C(8)	3.0832		4.080	.0270	.2465 1,4
C(1), C(10)	3.1081		4.080	.0270	.2213 1,4
C(1), H(16)	2.8329	2.7940	3.560	.0230	.1224 1,4
C(1), H(20)	2.6341	2.6030	3.560	.0230	.3160 1,4
C(2), C(5)	2.9527		4.080	.0270	.4178 1,4
C(2), H(17)	2.8085	2.7709	3.560	.0230	.1390 1,4
C(3), N(6)	2.9097		3.970	.0341	.4552 1,4
C(3), C(8)	3.2013		4.080	.0270	.1442 1,4
C(3), H(11)	2.8314	2.7923	3.560	.0230	.1236 1,4
C(4), H(13)	2.8178	2.7796	3.560	.0230	.1325 1,4
C(4), H(22)	2.8047	2.7709	3.560	.0230	.1389 1,4
C(4), H(23)	2.8226	2.7878	3.560	.0230	.1267 1,4
C(5), C(10)	2.9260		4.080	.0270	.4627 1,4
C(5), H(11)	2.8035	2.7631	3.560	.0230	.1449 1,4
C(5), H(21)	2.6924	2.6560	3.560	.0230	.2475 1,4
C(5), H(24)	2.8392	2.8010	3.560	.0230	.1177 1,4
N(6), C(9)	2.9316		3.970	.0341	.4160 1,4
N(6), H(13)	2.7858	2.7473	3.550	.0293	.1928 1,4
N(6), H(17)	2.7719	2.7329	3.550	.0293	.2078 1,4
N(6), H(23)	2.7913	2.7523	3.550	.0293	.1877 1,4
N(6), H(26)	2.8384	2.7981	3.550	.0293	.1458 1,4

S61

C(7), C(8)	2.8950	4.080	.0270	.5201	1,4
C(7), H(11)	2.7548	2.7155	3.560	.0230	.1853 1,4
C(7), H(12)	2.6527	2.6203	3.560	.0230	.2920 1,4
C(7), H(19)	2.6439	2.6105	3.560	.0230	.3054 1,4
C(7), H(24)	2.8507	2.8112	3.560	.0230	.1111 1,4
C(8), H(11)	2.8126	2.8184	3.560	.0230	.1065
C(8), H(18)	2.7527	2.7224	3.560	.0230	.1789 1,4
C(8), H(26)	2.8674	2.8271	3.560	.0230	.1012 1,4
C(9), H(19)	2.7574	2.7245	3.560	.0230	.1771 1,4
C(9), H(21)	2.8239	2.7861	3.560	.0230	.1279 1,4
C(10), H(23)	2.8526	2.8133	3.560	.0230	.1097 1,4
H(11), H(14)	2.4782	2.3965	3.240	.0200	.2393 1,4
H(11), H(23)	2.2418	2.3006	3.240	.0200	.3823
H(11), H(26)	2.2780	2.3363	3.240	.0200	.3224
H(12), H(13)	2.4576	2.3770	3.240	.0200	.2640 1,4
H(12), H(14)	2.5177	2.4306	3.240	.0200	.2007 1,4
H(12), H(20)	2.3547	2.3614	3.240	.0200	.2853
H(13), H(15)	2.4735	2.3922	3.240	.0200	.2446 1,4
H(14), H(15)	2.5452	2.4560	3.240	.0200	.1752 1,4
H(14), H(16)	2.4783	2.3968	3.240	.0200	.2390 1,4
H(15), H(17)	2.4613	2.3810	3.240	.0200	.2588 1,4
H(15), H(18)	2.5348	2.4468	3.240	.0200	.1841 1,4
H(16), H(18)	2.4865	2.4042	3.240	.0200	.2302 1,4
H(16), H(23)	2.3252	2.3883	3.240	.0200	.2495
H(17), H(19)	2.3943	2.3205	3.240	.0200	.3479 1,4
H(18), H(19)	2.5346	2.4450	3.240	.0200	.1859 1,4
H(18), H(22)	2.5312	2.5334	3.240	.0200	.1127
H(19), H(21)	2.4283	2.4277	3.240	.0200	.2038
H(19), H(22)	2.4864	2.4027	3.240	.0200	.2319 1,4
H(20), H(26)	2.4913	2.4086	3.240	.0200	.2250 1,4
H(20), H(27)	2.5325	2.4449	3.240	.0200	.1861 1,4
H(21), H(27)	2.4655	2.3850	3.240	.0200	.2537 1,4
H(22), H(24)	2.4598	2.3799	3.240	.0200	.2602 1,4
H(22), H(25)	2.5420	2.4531	3.240	.0200	.1780 1,4
H(23), H(25)	2.4682	2.3881	3.240	.0200	.2497 1,4
H(24), H(27)	2.4557	2.3767	3.240	.0200	.2645 1,4
H(25), H(26)	2.4623	2.3829	3.240	.0200	.2563 1,4
H(25), H(27)	2.5606	2.4698	3.240	.0200	.1625 1,4

BOND ANGLES, BENDING AND STRETCH-BEND ENERGIES (57 ANGLES)

$$EB = 0.021914(KB)(DT)(DT)(1+CF*DT+QF*DT**2+PF*DT**3+SF*DT**4)$$

$$DT = THETA-TZERO$$

$$CF = -1400.000E-5$$

$$QF = 5.600E-5$$

$$PF = -.070E-5$$

$$SF = .022E-6$$

$$ESB(J) = 2.51124(KSB(J))(DT)(DR1+DR2)$$

$$DR(I) = R(I) - R0(I)$$

$$EBDBD = -0.02191418(KBB1)(DT1)(KBB2)(DT2)$$

A T O M S				THETA	TZERO	KB	EB	KSB	ESB
C(2)- C(1)- N(6)	111.739	111.000	.780	.0092	.13	.0063			
C(2)- C(1)- H(11)	109.463	109.310	.590	.0003	.08	.0003			
C(2)- C(1)- H(12)	108.708	109.310	.590	.0047	.08	-.0014			
N(6)- C(1)- H(11)	110.752	109.300	.820	.0371	.08	.0048			
N(6)- C(1)- H(12)	109.452	109.300	.820	.0004	.08	.0006			
H(11)- C(1)- H(12)	106.572	107.600	.550	.0129					
C(1)- C(2)- C(3)	110.610	111.000	.670	.0022	.13	-.0022			
C(1)- C(2)- H(13)	109.476	109.310	.590	.0004	.08	.0004			
C(1)- C(2)- H(14)	110.202	109.310	.590	.0102	.08	.0022			
C(3)- C(2)- H(13)	109.497	109.310	.590	.0005	.08	.0004			
C(3)- C(2)- H(14)	110.137	109.310	.590	.0087	.08	.0016			
H(13)- C(2)- H(14)	106.839	107.600	.550	.0071					
C(2)- C(3)- C(4)	110.235	111.000	.670	.0087	.13	-.0041			
C(2)- C(3)- H(15)	110.039	109.310	.590	.0068	.08	.0015			
C(2)- C(3)- H(16)	109.812	109.310	.590	.0032	.08	.0009			
C(4)- C(3)- H(15)	110.071	109.310	.590	.0074	.08	.0018			
C(4)- C(3)- H(16)	110.029	109.310	.590	.0066	.08	.0016			
H(15)- C(3)- H(16)	106.590	107.600	.550	.0125					

S62

C(3)-C(4)-C(5)	113.130	111.000	.670	.0647	.13	.0181
C(3)-C(4)-H(17)	108.680	109.310	.590	.0052	.08	-.0016
C(3)-C(4)-H(18)	109.829	109.310	.590	.0035	.08	.0012
C(5)-C(4)-H(17)	108.855	109.310	.590	.0027	.08	-.0018
C(5)-C(4)-H(18)	109.887	109.310	.590	.0043	.08	.0022
H(17)-C(4)-H(18)	106.213	107.600	.550	.0237		
C(4)-C(5)-N(6)	109.795	108.000	.780	.0537	.13	.0217
C(4)-C(5)-C(8)	113.023	110.200	.670	.1124	.13	.0314
C(4)-C(5)-H(19)	107.333	109.800	.590	.0814	.08	-.0110
N(6)-C(5)-C(8)	110.829	108.000	.780	.1314	.13	.0346
N(6)-C(5)-H(19)	107.961	109.300	.820	.0328	.08	-.0069
C(8)-C(5)-H(19)	107.693	109.800	.590	.0591	.08	-.0096
C(1)-N(6)-C(5)	114.758	107.200	.720	.8087	.05	.0347
C(1)-N(6)-C(7)	113.030	107.200	.720	.4934	.05	.0235
C(5)-N(6)-C(7)	111.328	107.200	.720	.2536	.05	.0186
N(6)-C(7)-C(10)	113.137	111.000	.780	.0757	.13	.0199
N(6)-C(7)-H(20)	109.848	109.300	.820	.0053	.08	.0019
N(6)-C(7)-H(21)	108.810	109.300	.820	.0044	.08	-.0018
C(10)-C(7)-H(20)	110.022	109.310	.590	.0065	.08	.0021
C(10)-C(7)-H(21)	108.997	109.310	.590	.0013	.08	-.0010
H(20)-C(7)-H(21)	105.750	107.600	.550	.0423		
C(5)-C(8)-C(9)	111.078	111.000	.670	.0001	.13	.0007
C(5)-C(8)-H(22)	109.695	109.310	.590	.0019	.08	.0015
C(5)-C(8)-H(23)	110.860	109.310	.590	.0304	.08	.0055
C(9)-C(8)-H(22)	109.354	109.310	.590	.0000	.08	.0001
C(9)-C(8)-H(23)	109.459	109.310	.590	.0003	.08	.0003
H(22)-C(8)-H(23)	106.271	107.600	.550	.0217		
C(8)-C(9)-C(10)	110.967	111.000	.670	.0000	.13	-.0002
C(8)-C(9)-H(24)	109.334	109.310	.590	.0000	.08	.0001
C(8)-C(9)-H(25)	110.214	109.310	.590	.0104	.08	.0025
C(10)-C(9)-H(24)	109.335	109.310	.590	.0000	.08	.0001
C(10)-C(9)-H(25)	110.168	109.310	.590	.0094	.08	.0021
H(24)-C(9)-H(25)	106.722	107.600	.550	.0094		
C(7)-C(10)-C(9)	110.807	111.000	.670	.0005	.13	-.0014
C(7)-C(10)-H(26)	110.075	109.310	.590	.0075	.08	.0022
C(7)-C(10)-H(27)	109.951	109.310	.590	.0053	.08	.0020
C(9)-C(10)-H(26)	109.661	109.310	.590	.0016	.08	.0008
C(9)-C(10)-H(27)	109.891	109.310	.590	.0043	.08	.0015
H(26)-C(10)-H(27)	106.358	107.600	.550	.0189		

DIHEDRAL ANGLES, TORSIONAL ENERGY (ET) (90 ANGLES)

$$ET = (V1/2)(1+\cos(W)) + (V2/2)(1-\cos(2W)) + (V3/2)(1+\cos(3W))$$

$$ETS = -11.995 \cdot (R-R0) \cdot ((KTS1/2)(1+\cos(W)) + (KTS2/2)(1-\cos(2W)) + (KTS3/2)(1+\cos(3W)))$$

SIGN OF ANGLE A-B-C-D : WHEN LOOKING THROUGH B TOWARD C,
IF D IS COUNTERCLOCKWISE FROM A, NEGATIVE.

A T O M S		OMEGA	V1	V2	V3	ET	KTS3	ETS
C(1) C(2) C(3) C(4)	53.0	.185	.170	.520	.274	.059	.000	
C(1) C(2) C(3) H(15)	174.6	.000	.000	.280	.006	.059	.000	
C(1) C(2) C(3) H(16)	-68.4	.000	.000	.280	.013	.059	.000	
C(1) N(6) C(5) C(4)	-54.4	.958	-.155	.766	.672	.061	.000	
C(1) N(6) C(5) C(8)	71.2	.958	-.155	.766	.558	.061	-.001	
C(1) N(6) C(5) H(19)	-171.1	.072	-.012	.563	.030	.061	-.001	
C(1) N(6) C(7) C(10)	-73.1	.958	-.155	.766	.563	.061	-.001	
C(1) N(6) C(7) H(20)	50.3	.072	-.012	.563	.088	.061	-.001	
C(1) N(6) C(7) H(21)	165.6	.072	-.012	.563	.077	.061	-.002	
C(2) C(1) N(6) C(5)	56.8	.958	-.155	.766	.639	.061	.000	
C(2) C(1) N(6) C(7)	-174.1	.958	-.155	.766	.019	.061	.000	
C(2) C(3) C(4) C(5)	-53.0	.185	.170	.520	.274	.059	.000	
C(2) C(3) C(4) H(17)	68.0	.000	.000	.280	.012	.059	.000	
C(2) C(3) C(4) H(18)	-176.2	.000	.000	.280	.003	.059	.000	
C(3) C(2) C(1) N(6)	-54.7	-.302	.696	.499	.235	.059	.000	
C(3) C(2) C(1) H(11)	68.3	.000	.000	.280	.013	.059	.000	
C(3) C(2) C(1) H(12)	-175.6	.000	.000	.280	.004	.059	.000	
C(3) C(4) C(5) N(6)	52.4	-.302	.696	.499	.214	.059	.000	

C(3) C(4) C(5) C(8) -71.9 .185 .170 .520 .323 .059 -.001
C(3) C(4) C(5) H(19) 169.6 .000 .000 .280 .020 .059 -.001
C(4) C(3) C(2) H(13) -67.8 .000 .000 .280 .011 .059 .000
C(4) C(3) C(2) H(14) 175.0 .000 .000 .280 .005 .059 .000
C(4) C(5) N(6) C(7) 175.6 .958 -.155 .766 .010 .061 .000
C(4) C(5) C(8) C(9) -179.5 .185 .170 .520 .000 .059 .000
C(4) C(5) C(8) H(22) -58.5 .000 .000 .280 .000 .059 .000
C(4) C(5) C(8) H(23) 58.6 .000 .000 .280 .000 .059 .000
C(5) C(4) C(3) H(15) -174.6 .000 .000 .280 .006 .059 .000
C(5) C(4) C(3) H(16) 68.2 .000 .000 .280 .013 .059 .000
C(5) N(6) C(1) H(11) -65.6 .072 -.012 .563 .053 .061 .000
C(5) N(6) C(1) H(12) 177.2 .072 -.012 .563 .003 .061 .000
C(5) N(6) C(7) C(10) 57.8 .958 -.155 .766 .626 .061 .000
C(5) N(6) C(7) H(20) -178.8 .072 -.012 .563 .001 .061 .000
C(5) N(6) C(7) H(21) -63.5 .072 -.012 .563 .047 .061 .000
C(5) C(8) C(9) C(10) -52.7 .185 .170 .520 .275 .059 .000
C(5) C(8) C(9) H(24) 68.0 .000 .000 .280 .012 .059 .000
C(5) C(8) C(9) H(25) -175.0 .000 .000 .280 .005 .059 .000
N(6) C(1) C(2) H(13) 66.0 .000 .000 .374 .009 .059 .000
N(6) C(1) C(2) H(14) -176.8 .000 .000 .374 .003 .059 .000
N(6) C(5) C(4) H(17) -68.5 .000 .000 .374 .018 .059 -.001
N(6) C(5) C(4) H(18) 175.6 .000 .000 .374 .005 .059 .000
N(6) C(5) C(8) C(9) 56.8 -.302 .696 .499 .257 .059 .000
N(6) C(5) C(8) H(22) 177.8 .000 .000 .374 .001 .059 .000
N(6) C(5) C(8) H(23) -65.2 .000 .000 .374 .007 .059 .000
N(6) C(7) C(10) C(9) -53.3 -.302 .696 .499 .222 .059 .000
N(6) C(7) C(10) H(26) 68.1 .000 .000 .374 .017 .059 .000
N(6) C(7) C(10) H(27) -175.0 .000 .000 .374 .006 .059 .000
C(7) N(6) C(1) H(11) 63.6 .072 -.012 .563 .047 .061 .000
C(7) N(6) C(1) H(12) -53.6 .072 -.012 .563 .065 .061 .000
C(7) N(6) C(5) C(8) -58.8 .958 -.155 .766 .615 .061 .000
C(7) N(6) C(5) H(19) 58.9 .072 -.012 .563 .046 .061 .000
C(7) C(10) C(9) C(8) 50.4 .185 .170 .520 .285 .059 .000
C(7) C(10) C(9) H(24) -70.3 .000 .000 .280 .020 .059 .000
C(7) C(10) C(9) H(25) 172.7 .000 .000 .280 .010 .059 .000
C(8) C(5) C(4) H(17) 167.2 .000 .000 .280 .030 .059 -.001
C(8) C(5) C(4) H(18) 51.3 .000 .000 .280 .014 .059 -.001
C(8) C(9) C(10) H(26) -71.4 .000 .000 .280 .024 .059 -.001
C(8) C(9) C(10) H(27) 172.1 .000 .000 .280 .012 .059 .000
C(9) C(8) C(5) H(19) -61.1 .000 .000 .280 .000 .059 .000
C(9) C(10) C(7) H(20) -176.6 .000 .000 .280 .002 .059 .000
C(9) C(10) C(7) H(21) 67.9 .000 .000 .280 .012 .059 .000
C(10) C(9) C(8) H(22) -173.9 .000 .000 .280 .007 .059 .000
C(10) C(9) C(8) H(23) 70.0 .000 .000 .280 .019 .059 -.001
H(11) C(1) C(2) H(13) -170.9 .000 .000 .238 .013 .059 .000
H(11) C(1) C(2) H(14) -53.7 .000 .000 .238 .006 .059 .000
H(12) C(1) C(2) H(13) -54.9 .000 .000 .238 .004 .059 .000
H(12) C(1) C(2) H(14) 62.3 .000 .000 .238 .001 .059 .000
H(13) C(2) C(3) H(15) 53.8 .000 .000 .238 .006 .059 .000
H(13) C(2) C(3) H(16) 170.9 .000 .000 .238 .013 .059 .000
H(14) C(2) C(3) H(15) -63.4 .000 .000 .238 .002 .059 .000
H(14) C(2) C(3) H(16) 53.7 .000 .000 .238 .007 .059 .000
H(15) C(3) C(4) H(17) -53.6 .000 .000 .238 .007 .059 .000
H(15) C(3) C(4) H(18) 62.2 .000 .000 .238 .001 .059 .000
H(16) C(3) C(4) H(17) -170.8 .000 .000 .238 .014 .059 .000
H(16) C(3) C(4) H(18) -55.0 .000 .000 .238 .004 .059 .000
H(17) C(4) C(5) H(19) 48.6 .000 .000 .238 .020 .059 -.001
H(18) C(4) C(5) H(19) -67.3 .000 .000 .238 .009 .059 .000
H(19) C(5) C(8) H(22) 59.9 .000 .000 .238 .000 .059 .000
H(19) C(5) C(8) H(23) 177.0 .000 .000 .238 .002 .059 .000
H(20) C(7) C(10) H(26) -55.1 .000 .000 .238 .004 .059 .000
H(20) C(7) C(10) H(27) 61.7 .000 .000 .238 .000 .059 .000
H(21) C(7) C(10) H(26) -170.7 .000 .000 .238 .014 .059 -.001
H(21) C(7) C(10) H(27) -53.8 .000 .000 .238 .006 .059 .000
H(22) C(8) C(9) H(24) -53.3 .000 .000 .238 .007 .059 .000
H(22) C(8) C(9) H(25) 63.8 .000 .000 .238 .002 .059 .000
H(23) C(8) C(9) H(24) -169.3 .000 .000 .238 .018 .059 -.001
H(23) C(8) C(9) H(25) -52.3 .000 .000 .238 .010 .059 .000
H(24) C(9) C(10) H(26) 168.0 .000 .000 .238 .023 .059 -.001
H(24) C(9) C(10) H(27) 51.4 .000 .000 .238 .012 .059 .000
H(25) C(9) C(10) H(26) 51.0 .000 .000 .238 .013 .059 .000

S64

H(25) C(9) C(10) H(27) -65.6 .000 .000 .238 .005 .059 .000

=====

NORMAL MODE VIBRATIONAL ANALYSIS

=====

Molecular Shape : ASYMMETRIC ROTOR WITH KAPPA = -.696033
 Symmetry Point Group : C1
 Symmetry Number : 1
 Chirality : yes

0 FUNDAMENTAL NORMAL VIBRATIONAL FREQUENCIES
 (THEORETICALLY 75 VALUES)

Frequency : in 1/cm

A(i) : IR intensity (vs,s,m,w,vw,-- or in 10**6 cm/mole)

A(i) = -- : IR inactive

no	Frequency	Symmetry	A(i)
1.	2946.0	(A)	m
2.	2940.7	(A)	m
3.	2935.3	(A)	m
4.	2933.4	(A)	s
5.	2929.9	(A)	m
6.	2927.1	(A)	m
7.	2926.2	(A)	m
8.	2917.8	(A)	m
9.	2916.9	(A)	m
10.	2894.2	(A)	m
11.	2890.7	(A)	m
12.	2887.1	(A)	m
13.	2882.3	(A)	m
14.	2876.9	(A)	m
15.	2870.0	(A)	m
16.	2869.7	(A)	w
17.	2801.1	(A)	m
18.	1589.0	(A)	w
19.	1568.3	(A)	w
20.	1527.0	(A)	w
21.	1492.4	(A)	w
22.	1480.8	(A)	w
23.	1475.6	(A)	w
24.	1472.5	(A)	w
25.	1468.6	(A)	w
26.	1467.0	(A)	w
27.	1461.1	(A)	w
28.	1447.3	(A)	w
29.	1440.1	(A)	w
30.	1428.6	(A)	w
31.	1414.9	(A)	w
32.	1402.6	(A)	w
33.	1392.3	(A)	w
34.	1373.3	(A)	w
35.	1357.3	(A)	m
36.	1346.5	(A)	w
37.	1324.7	(A)	w
38.	1251.7	(A)	w
39.	1228.6	(A)	w
40.	1219.4	(A)	w
41.	1215.9	(A)	w
42.	1206.7	(A)	w
43.	1201.1	(A)	w
44.	1162.2	(A)	w
45.	1143.9	(A)	w
46.	1087.2	(A)	w

47.	1054.7	(A)	w
48.	1044.7	(A)	w
49.	1041.0	(A)	w
50.	1008.6	(A)	w
51.	992.9	(A)	w
52.	956.6	(A)	w
53.	938.4	(A)	w
54.	913.4	(A)	w
55.	886.7	(A)	w
56.	864.9	(A)	w
57.	859.1	(A)	w
58.	840.4	(A)	w
59.	823.4	(A)	w
60.	816.5	(A)	w
61.	794.1	(A)	w
62.	743.0	(A)	w
63.	596.2	(A)	w
64.	574.0	(A)	w
65.	510.2	(A)	w
66.	448.6	(A)	w
67.	421.9	(A)	w
68.	382.2	(A)	w
69.	361.7	(A)	w
70.	345.9	(A)	w
71.	306.9	(A)	w
72.	294.8	(A)	w
73.	194.8	(A)	vw
74.	178.6	(A)	w
75.	145.6	(A)	w
76.	(.0)	(t/r)	
77.	(.0)	(t/r)	
78.	(.0)	(t/r)	
79.	(.0)	(t/r)	
80.	(.0)	(t/r)	
81.	(.0)	(t/r)	

=====

STATISTICAL THERMODYNAMICS ANALYSIS

=====

Structure name : MMX chinolys
Temperature : 298.16 K
Symmetry number : 1
Optical isomers : 2
Zero Point Energy : 154.865 Kcal/mol

	ENERGY	ENTHALPY	ENTROPY	FREE ENERGY	HEAT CAPACITY
	(Kcal/mol)	(Kcal/mol)	(eu)	(Kcal/mol)	(cal/mol/deg)
Translational	.889	1.481	40.684	-10.649	4.967
Rotational	.889	.889	29.262	-7.836	2.980
Vibrational	158.609%	158.609%	19.665*	152.746%	31.455*
Potential	22.393#	22.393#	.000	22.393#	.000
Mixing	.000	.000	1.377	-.411	.000
Total	182.779	183.371	90.988	156.242	39.403

Enthalpy Function (H-Ho)/T = 20.51 cal/mol/deg
Free Energy Function -(G-Ho)/T = 70.48 cal/mol/deg

% Includes zero point energy (ZPE).
* Excludes contribution from frequencies lower than 40 (1/cm).
Includes steric energy (SE).
Internal rotation contributions are not considered

This structure has 0 imaginary frequencies,
0 free internal rotation (fir) frequencies
(>= 0, < 10 /cm),
0 restricted internal rotation (rir) frequencies
(>= 10, < 40 /cm),
6 zero frequencies, and

75 real frequencies.

FINAL STERIC ENERGY IS 22.3925 KCAL/MOL.

```

COMPRESSION      .7469
BENDING          2.5268
BEND-BEND        -.1114
STRETCH-BEND     .2084
VANDERWAALS
  1,4 ENERGY    11.6197
  OTHER          .3508

TORSIONAL        7.0788
TORSION-STRETCH  -.0275
DIPOLE-DIPOLE    .0000
CHARGE-DIPOLE    .0000
CHARGE-CHARGE    .0000
  
```

COORDINATES TRANSLATED TO NEW ORIGIN WHICH IS CENTER OF MASS

```

C( 1)  .68532  1.35073  .45088  ( 1)
C( 2)  2.17026  .98612  .42379  ( 1)
C( 3)  2.35209  -.53314  .43216  ( 1)
C( 4)  1.53276 -1.17101  -.69411  ( 1)
C( 5)  .05374  -.75523  -.67458  ( 1)
N( 6)  -.05076  .70884  -.64019  ( 8)
C( 7)  -1.44542  1.14516  -.72454  ( 1)
C( 8)  -.73292 -1.38666  .48506  ( 1)
C( 9)  -2.20371  -.95250  .45485  ( 1)
C(10)  -2.32372  .57417  .39404  ( 1)
H(11)  .24836  1.06751  1.44663  ( 5)
H(12)  .58745  2.45634  .36406  ( 5)
H(13)  2.64075  1.41197  -.49223  ( 5)
H(14)  2.69378  1.43984  1.29620  ( 5)
H(15)  3.43018  -.78940  .31323  ( 5)
H(16)  2.03384  -.94595  1.41625  ( 5)
H(17)  1.97781  -.87346  -1.67207  ( 5)
H(18)  1.61519  -2.28044  -.63963  ( 5)
H(19)  -.40428  -1.11071  -1.62849  ( 5)
H(20)  -1.49457  2.25684  -.71765  ( 5)
H(21)  -1.86111  .83040  -1.70808  ( 5)
H(22)  -.67431  -2.49716  .41777  ( 5)
H(23)  -.28505  -1.10984  1.46434  ( 5)
H(24)  -2.70166  -1.39770  -.43760  ( 5)
H(25)  -2.73940  -1.34466  1.34986  ( 5)
H(26)  -2.02779  1.01245  1.37367  ( 5)
H(27)  -3.38655  .86456  .22859  ( 5)
  
```

MOMENT OF INERTIA WITH THE PRINCIPAL AXES

(1) UNIT = 10**(-39) GM*CM**2
 IX= 36.4092 IY= 73.9026 IZ= 90.6290

(2) UNIT = AU A**2
 IX= 219.2853 IY= 445.1005 IZ= 545.8402

DIPOLE MOMENT = .549 D

COMPONENTS WITH PRINCIPAL AXES

X = .2577 Y = .1773 Z = -.4516

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.747890	-.577020	.451832
2	6	0	1.742621	.881522	-.005301
3	6	0	.340123	1.462609	.174458
4	6	0	.769647	-1.389923	-.400441
5	6	0	-.694849	.668200	-.628628
6	7	0	-.560894	-.807686	-.520659
7	6	0	-2.051959	.526756	.091692
8	6	0	-1.505328	-.817436	.614671
9	1	0	2.751562	-1.012635	.372000
10	1	0	2.474379	1.469570	.560588
11	1	0	2.038912	.935329	-1.062506
12	1	0	.299246	2.517255	-.125503
13	1	0	1.182518	-1.477745	-1.415498
14	1	0	.653690	-2.410119	-.014451
15	1	0	-.709506	1.014722	-1.671862
16	1	0	-2.308432	1.295826	.824927

S68

17	1	0	1.462939	-0.624533	1.511075
18	1	0	.087181	1.430040	1.242783
19	1	0	-2.879904	.384505	-.605771
20	1	0	-2.179647	-1.681141	.633320
21	1	0	-1.035541	-.715511	1.605814

Rotational constants (GHZ): 3.4272052 2.0718930 1.5458387

Isotopes: C-12,C-12,C-12,C-12,C-12,N-14,C-12,C-12,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1

Dipole moment (Debye):

X= .4162 Y= .6151 Z= .8584 Tot= 1.1351

Quadrupole moment (Debye-Ang):

XX= -50.6904 YY= -51.2558 ZZ= -51.8365

XY= -1.0934 XZ= -1.3122 YZ= -1.5719

Octapole moment (Debye-Ang**2):

XXX= -3.0345 YYY= -2.1643 ZZZ= -.0982 XYY= .4381

XXY= -1.3615 XXZ= -.5378 XZZ= .7760 YZZ= 2.0091

YYZ= 1.3829 XYZ= 2.1506

Hexadecapole moment (Debye-Ang**3):

XXXX= -673.3675 YYYY= -393.8985 ZZZZ= -161.0196 XXXY= 1.0797

XXXZ= 3.3091 YYYY= .3126 YYYZ= -3.6598 ZZZX= -2.1879

ZZZY= -1.5635 XYY= -178.8571 XXZZ= -141.2090 YYZZ= -96.3237

XXYZ= 1.0250 YYXZ= -2.6514 ZZXY= -2.2851

N-N= 4.075894165805D+02 E-N=-1.576980450427D+03 KE= 3.266508941426D+02

1\1\GINC-ARMON\FOpt\RMP2-FC\6-31G(d)\C7H13N1\BELOSTOT\16-Oct-2002\0\#

MP2/6-31G* OPT=(NEWTON, CARTESIAN) GEOM=ALLCHECKPOINT GUESS=CHECKPOIN

T\Azabicyclo[4.2.0]octane, mimimum 1; cis geometry\0,1\C,-1.67251998

34,0.6165159886,-0.6440557988\C,-1.6482973786,0.5627633165,0.883317492

5\C,-0.1992760311,0.6117303002,1.3679978789\C,-0.9252136908,-0.5910844

785,-1.2162214786\C,0.61391941,-0.5555494244,0.799341918\N,0.398707108

1,-0.8115701244,-0.6484078759\C,2.0661638859,-0.1745635863,0.443742682

9\C,1.5309844157,0.0763367724,-0.9809661807\H,-2.701987325,0.622492735

2,-1.023072534\H,-2.2217526047,1.3931186267,1.3112906533\H,-2.12757295

27,-0.3656223587,1.2250201583\H,-0.1398394197,0.5945931307,2.463488653

2\H,-1.5210876859,-1.4938359938,-1.0200296837\H,-0.8127544571,-0.51406

26167,-2.3046392632\H,0.462686394,-1.4549041078,1.4132793363\H,2.50511

10616,0.6693186877,0.9823244608\H,-1.203554823,1.5506691999,-0.9800307

076\H,0.2409964703,1.5645773437,1.0445772702\H,2.7412659368,-1.0320042

04,0.4786222335\H,2.1351826322,-0.2617525349,-1.8304838729\H,1.2577932

509,1.1315096323,-1.1404306581\Version=IBM-RS6000-G98RevA.7\HF=-327.0

549918\MP2=-328.1310299\RMSD=4.767e-09\RMSF=9.271e-06\Dipole=-0.090558

2,0.3816204,0.1230287\PG=C01 [X(C7H13N1)]\@

Conformer 2

Item Value Threshold Converged?
 Maximum Force .000113 .000450 YES
 RMS Force .000035 .000300 YES
 Maximum Displacement .001399 .001800 YES
 RMS Displacement .000491 .001200 YES
 Predicted change in Energy=-1.514288D-07
 Optimization completed.

-- Stationary point found.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.372212	-1.116345	-.773709
2	6	0	-1.402184	-1.070978	.751917
3	6	0	.028012	-1.087737	1.286975
4	6	0	-.658983	.119624	-1.300402
5	6	0	.926585	-.065439	.609338
6	7	0	.751030	.148200	-.875970
7	6	0	.818369	1.450026	.853226
8	6	0	1.177213	1.568972	-.639611
9	1	0	-.844739	-2.016836	-1.112291
10	1	0	-1.924674	-.160610	1.074203
11	1	0	-1.962559	-1.919062	1.162080
12	1	0	.055515	-.925794	2.372406
13	1	0	-.669012	.147567	-2.396685
14	1	0	-1.226136	1.004691	-.955415
15	1	0	1.973869	-.366404	.751923
16	1	0	-.209534	1.767484	1.052487
17	1	0	-2.387483	-1.155036	-1.185360
18	1	0	.448324	-2.085463	1.105926
19	1	0	1.483887	1.904424	1.594487
20	1	0	2.254931	1.669455	-.807867
21	1	0	.649603	2.309456	-1.250497

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.694550	.923659	-.056332
2	6	0	-1.788185	-.503889	.476426
3	6	0	-.862891	-1.408472	-.334492
4	6	0	-.271430	1.432747	.114780
5	6	0	.541418	-.843783	-.478572
6	7	0	.680836	.646044	-.687330
7	6	0	1.554600	-.789574	.678300
8	6	0	1.989790	.543654	.042223
9	1	0	-1.967416	.946593	-1.118767
10	1	0	-1.503593	-.511122	1.536893
11	1	0	-2.816459	-.879718	.422518
12	1	0	-.801777	-2.415806	.097582
13	1	0	-.181558	2.477471	-.206455
14	1	0	-.037290	1.412130	1.195880
15	1	0	1.026042	-1.318963	-1.342897
16	1	0	1.071391	-.640415	1.648521
17	1	0	-2.386033	1.587402	.475667
18	1	0	-1.290595	-1.521316	-1.339098
19	1	0	2.287566	-1.598496	.763540
20	1	0	2.809235	.421718	-.674383
21	1	0	2.212134	1.392169	.698315

Rotational constants (GHZ): 3.4269775 2.0683646 1.5467217

Isotopes: C-12,C-12,C-12,C-12,C-12,N-14,C-12,C-12,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1

Dipole moment (Debye):

X= -1.299 Y= -0.7041 Z= 1.2773 Tot= 1.4643
 Quadrupole moment (Debye-Ang):
 XX= -49.6369 YY= -50.6141 ZZ= -53.2263
 XY= -0.7466 XZ= 0.9779 YZ= 2.0456
 Octapole moment (Debye-Ang**2):
 XXX= 4.3927 YYY= 1.9498 ZZZ= 2.0992 XYY= 0.7048
 XXY= 0.0154 XXZ= -1.5400 XZZ= -1.3520 YZZ= -2.4209
 YYZ= 0.8861 XYZ= 1.3987
 Hexadecapole moment (Debye-Ang**3):
 XXXX= -667.9053 YYYY= -393.6667 ZZZZ= -164.5451 XXXY= 1.2760
 XXXZ= -4.2713 YYYY= -1.7127 YYYZ= -0.6802 ZZZX= 2.7115
 ZZZY= 4.9849 XYY= -177.3645 XXZZ= -140.9000 YYZZ= -96.1069
 XXYZ= 3.1013 YYXZ= 0.8092 ZZXY= -1.9928
 N-N= 4.073404491776D+02 E-N= -1.576445205291D+03 KE= 3.266537833581D+02
 1\1\GINC-ARMON\FOpt\RMP2-FC\6-31G(d)\C7H13N1\BELOSTOT\17-Oct-2002\0\#\n#
 OPT=(NEWTON, CARTESIAN) MP2/6-31G* GEOM=ALLCHECKPOINT GUESS=CHECKPOIN
 T\Azabicyclo[4.2.0]octane, minimum 2; cis geometry\0,1\C,-1.37221180
 13,-1.1163452703,-0.7737094844\C,-1.4021842813,-1.070978126,0.75191650
 14\C,0.0280118278,-1.0877374396,1.2869745667\C,-0.6589826383,0.1196236
 11,-1.3004019086\C,0.9265848124,-0.065438988,0.6093380774\N,0.75103002
 29,0.1481995096,-0.8759704799\C,0.8183687119,1.4500263987,0.8532262382
 \C,1.1772128481,1.5689716131,-0.6396112036\H,-0.8447387166,-2.01683602
 03,-1.1122907889\H,-1.9246739422,-0.1606101364,1.0742033928\H,-1.96255
 91495,-1.919062017,1.1620800134\H,0.0555148923,-0.9257937726,2.3724062
 667\H,-0.669011741,0.1475673404,-2.3966850053\H,-1.2261357676,1.004691
 3996,-0.9554147751\H,1.9738686837,-0.3664044253,0.7519225523\H,-0.2095
 33502,1.7674838101,1.052486594\H,-2.3874825881,-1.1550357169,-1.185360
 1349\H,0.4483241114,-2.0854631077,1.1059257156\H,1.4838867556,1.904424
 2207,1.5944871966\H,2.2549313558,1.669454583,-0.8078672449\H,0.6496025
 721,2.3094564832,-1.2504971463\\Version=IBM-RS6000-G98RevA.7\HF=-327.0
 463378\MP2=-328.1239711\RMSD=5.045e-09\RMSF=3.511e-05\Dipole=-0.291977
 ,0.217435,0.3959366\PG=C01 [X(C7H13N1)]\@

Conformation 3

[illegible]

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.849681	0.079410	-0.708040
2	6	0	-1.843594	0.170104	0.831533
3	6	0	-0.411918	0.109792	1.395601
4	6	0	-0.557660	0.637967	-1.295144
5	6	0	-0.454451	-0.770608	0.508929
6	7	0	0.533887	-0.246184	-0.888647
7	6	0	1.976674	-0.563154	0.631884
8	6	0	1.849988	0.359646	-0.594668
9	1	0	-1.927888	-0.966618	-1.025105
10	1	0	-2.321833	1.102055	1.154586
11	1	0	-2.443784	-0.647096	1.247237
12	1	0	0.022900	1.117034	1.420586
13	1	0	-0.605138	0.678348	-2.390100
14	1	0	-0.403619	1.674432	-0.940390
15	1	0	0.106183	-1.812269	0.552304
16	1	0	2.338865	-0.116218	1.561819
17	1	0	-2.719049	0.601902	-1.121258
18	1	0	-0.408217	-0.256749	2.429251
19	1	0	2.542588	-1.472907	0.420034
20	1	0	2.591275	0.258811	-1.395189
21	1	0	1.780946	1.423621	-0.313815

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.852563	0.631787	-0.312731
2	6	0	-1.842570	-0.835206	0.163062
3	6	0	-0.408646	-1.339448	0.410268
4	6	0	-0.642743	1.390119	0.223237
5	6	0	0.548643	-0.666426	-0.560570
6	7	0	0.551004	0.819733	-0.399711
7	6	0	2.036022	-0.673543	-0.156879
8	6	0	1.787547	0.738180	0.406446
9	1	0	-1.807567	0.675005	-1.406774
10	1	0	-2.426189	-0.934635	1.085618
11	1	0	-2.336178	-1.464731	-0.585872
12	1	0	-0.097789	-1.095582	1.434047
13	1	0	-0.705288	2.457869	-0.019270
14	1	0	-0.610946	1.311047	1.326222
15	1	0	0.328499	-0.981592	-1.590346
16	1	0	2.350838	-1.447797	0.548201
17	1	0	-2.782360	1.127394	-0.013735
18	1	0	-0.350960	-2.430834	0.318899
19	1	0	2.705083	-0.672728	-1.020099
20	1	0	2.527824	1.517035	0.192242
21	1	0	1.593869	0.728650	1.491844

Rotational constants (GHz): 3.6952135 1.9708554 1.4812835
Isotopes: C-12,C-12,C-12,C-12,C-12,N-14,C-12,C-12,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1

Dipole moment (Debye):

X= -0.2168 Y= -0.7863 Z= 0.8824 Tot= 1.2017

Quadrupole moment (Debye-Ang):

XX= -50.0026 YY= -51.4420 ZZ= -51.8226

XY= -0.9101 XZ= 0.6551 YZ= 1.7153

Octapole moment (Debye-Ang**2):

XXX= 3.7454 YYY= 1.2089 ZZZ= 0.0226 XYY= -0.4065

XXY= 2.1133 XXZ= -0.3820 XZZ= -0.3656 YZZ= -2.0843

YYZ= 0.6860 XYZ= 0.5121

Hexadecapole moment (Debye-Ang**3):

XXXX= -730.3354 YYYY= -379.1240 ZZZZ= -143.7426 XXXY= 0.6550

XXXZ= -6.4344 YYYY= -0.9780 YYYZ= 1.0165 ZZZX= 0.3386

ZZZY= 2.3498 XXYY= -184.6548 XXZZ= -144.5027 YYZZ= -92.3704

XXYZ= 1.3514 YYXZ= 2.8411 ZZZY= -1.3085

N-N= 4.068624702477D+02 E-N=-1.575537129557D+03 KE= 3.266508338709D+02

1\1\GINC-ILANIT\FOpt\RMP2-FC\6-31G(d)\C7H13N1\BELOSTOT\17-Oct-2002\0\

OPT=(NEWTON, CARTESIAN) MP2/6-31G*\Azabicyclo[4.2.0]octane, 1,4-twi

st stable conformer of cis geometry\0,1\C,-1.8496808256,0.0794102731,

-0.7080397684\C,-1.843594101,0.1701042845,0.8315331583\C,-0.4119180335

,0.1097921274,1.3956009893\C,-0.557659559,0.6379669507,-1.2951439648\C

,0.4544514269,-0.7706075194,0.5089294711\N,0.5338865403,-0.2461844082,

-0.8886474469\C,1.9766738027,-0.5631541057,0.6318839177\C,1.8499880397

,0.3596455503,-0.5946682814\H,-1.9278881727,-0.9666179781,-1.025104951

9\H,-2.3218327209,1.1020545897,1.1545858513\H,-2.4437838711,-0.6470955

411,1.2472370622\H,0.0228999095,1.1170340184,1.4205855504\H,-0.6051378

568,0.6783477875,-2.3900996392\H,-0.4036189292,1.6744320091,-0.9403903

977\H,0.1061833917,-1.8122693249,0.5523035378\H,2.3388652667,-0.116217

7362,1.5618194292\H,-2.7190492206,0.6019021697,-1.1212582873\H,-0.4082

173888,-0.256749261,2.4292512681\H,2.5425878712,-1.4729074939,0.420033

5528\H,2.5912754856,0.258810912,-1.395188831\H,1.7809459526,1.42362134

06,-0.3138151468\Version=SGI64-G98RevA.7\HF=-327.0511676\MP2=-328.127

2762\RMSD=7.910e-09\RMSF=1.626e-05\Dipole=-0.0726283,0.2433911,0.35286

36\PG=C01 [X(C7H13N1)]\@

Conformation 4

Item Value Threshold Converged?
 Maximum Force .000091 .000450 YES
 RMS Force .000026 .000300 YES
 Maximum Displacement .001236 .001800 YES
 RMS Displacement .000459 .001200 YES
 Predicted change in Energy=-7.832062D-08

Optimization completed.

-- Stationary point found.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.714144	.743048	-.724752
2	6	0	-1.717707	.693745	.814515
3	6	0	-.306854	.757261	1.431655
4	6	0	-.769692	-.290592	-1.353040
5	6	0	.487107	-.319016	.728933
6	7	0	.509398	-.067599	-.714942
7	6	0	2.008867	-.537971	.643844
8	6	0	1.709930	-.912795	-.830395
9	1	0	-2.735559	.597334	-1.097452
10	1	0	-2.342038	1.507897	1.201246
11	1	0	-2.191787	-.242931	1.138135
12	1	0	.157506	1.731304	1.239952
13	1	0	-1.145850	-1.319460	-1.183771
14	1	0	-.690840	-.134796	-2.435555
15	1	0	.019276	-1.304469	.947331
16	1	0	2.564960	.399805	.714496
17	1	0	-1.384387	1.735206	-1.052719
18	1	0	-.354569	.604889	2.517081
19	1	0	2.453535	-1.297967	1.290396
20	1	0	1.482185	-1.989186	-.926474
21	1	0	2.416741	-.616509	-1.612630

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.834055	-.769536	-.244400
2	6	0	-1.886683	.703306	.202541
3	6	0	-.634632	1.508590	-.196569
4	6	0	-.540832	-1.477113	.182282
5	6	0	.539050	.698741	.302612
6	7	0	.527943	-.633994	-.307450
7	6	0	2.031983	.778597	-.065772
8	6	0	1.963455	-.769026	-.007394
9	1	0	-2.705874	-1.303543	.153338
10	1	0	-2.790042	1.172938	-.204376
11	1	0	-1.982991	.738674	1.296304
12	1	0	-.567340	1.607505	-1.285985
13	1	0	-.504804	-1.597765	1.283581
14	1	0	-.479321	-2.475041	-.267922
15	1	0	.471708	.622519	1.410464
16	1	0	2.186208	1.135087	-1.086941
17	1	0	-1.891982	-.816635	-1.337608
18	1	0	-.668806	2.514418	.240220
19	1	0	2.703072	1.292700	.626102
20	1	0	2.166398	-1.135676	1.014418
21	1	0	2.538461	-1.358575	-.729238

Rotational constants (GHZ): 3.6704882 1.9512668 1.3912041

Isotopes: C-12,C-12,C-12,C-12,C-12,N-14,C-12,C-12,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1

Dipole moment (Debye):

X= .0992 Y= .0971 Z= .7312 Tot= .7443
 Quadrupole moment (Debye-Ang):
 XX= -49.8291 YY= -50.5347 ZZ= -52.0252
 XY= .1537 XZ= .3729 YZ= -.3236
 Octapole moment (Debye-Ang**2):
 XXX= 3.7974 YYY= -3.3959 ZZZ= -.5035 XYY= .5958
 XXY= -1.2733 XXZ= -1.0767 XZZ= .6810 YZZ= .8412
 YYZ= -.7142 XYZ= .5726
 Hexadecapole moment (Debye-Ang**3):
 XXXX= -768.0619 YYYY= -415.3601 ZZZZ= -119.0617 XXXY= -1.9407
 XXXZ= -.1533 YYYY= -.5459 YYYZ= 5.2686 ZZZX= -.0007
 ZZZY= -1.2954 XXYY= -195.8334 XXZZ= -146.0792 YYZZ= -89.6911
 XXYZ= .1821 YYXZ= -.7582 ZZXY= .5836
 N-N= 4.048779823461D+02 E-N=-1.571566038630D+03 KE= 3.266550203990D+02
 1\1\GINC-ESHEL\FOpt\RMP2-FC\6-31G(d)\C7H13N1\BELOSTOT\16-Oct-2002\0\#\n
 MP2/6-31G* OPT=(NEWTON, CARTESIAN) GEOM=ALLCHECKPOINT GUESS=CHECKPOIN
 T\Azabicyclo[4.2.0]octane, minimum 3; trans geometry\0,1\C,-1.714143
 6367,0.7430481215,-0.7247519742\C,-1.7177071855,0.6937451392,0.8145154
 68\C,-0.3068541961,0.7572614346,1.4316549924\C,-0.769692276,-0.2905924
 96,-1.3530404094\C,0.4871070068,-0.319016441,0.7289326333\N,0.50939822
 48,-0.0675992214,-0.714942227\C,2.0088666323,-0.5379711422,0.643844460
 6\C,1.7099303211,-0.9127947994,-0.8303952998\H,-2.7355591932,0.5973337
 736,-1.097451801\H,-2.3420378808,1.5078969193,1.2012464419\H,-2.191787
 3735,-0.2429310899,1.1381348744\H,0.1575064737,1.7313041961,1.23995249
 29\H,-1.1458496032,-1.3194600443,-1.1837714179\H,-0.6908402211,-0.1347
 962685,-2.43555513\H,0.0192759977,-1.3044694855,0.9473306871\H,2.56496
 00289,0.3998047583,0.7144963457\H,-1.3843870557,1.7352058451,-1.052719
 3728\H,-0.3545690012,0.6048886485,2.5170810469\H,2.453534641,-1.297967
 1743,1.2903960689\H,1.4821845093,-1.9891858704,-0.9264737956\H,2.41674
 11086,-0.6165085591,-1.6126300769\Version=IBM-RS6000-G98RevA.7\HF=-32
7.052606\MP2=-328.1299048RMSD=5.283e-09\RMSF=2.648e-05\Dipole=-0.0774
 413,-0.210241,0.0831491\PG=C01 [X(C7H13N1)]\@\n

Conformation 5 (RI transition state)

Item	Value	Threshold	Converged?
Maximum Force	.000001	.000450	YES
RMS Force	.000000	.000300	YES
Maximum Displacement	.000071	.001800	YES
RMS Displacement	.000022	.001200	YES
Predicted change in Energy=-2.324948D-11			

Optimization completed.

```
-- Stationary point found.
```

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.756618	.680125	-.793457
2	6	0	-1.741422	.630062	.741895
3	6	0	-.315219	.681993	1.281322
4	6	0	-.535609	.032427	-1.505867
5	6	0	.360000	-.595612	.822875
6	7	0	.385653	-.739918	-.658326
7	6	0	1.898861	-.631155	.825850
8	6	0	1.808419	-.343563	-.682889
9	1	0	-2.680875	.219225	-1.155740
10	1	0	-2.353842	1.447432	1.138522
11	1	0	-2.201263	-.302516	1.092781
12	1	0	.216088	1.560291	.888759
13	1	0	-.894802	-.617477	-2.312985
14	1	0	.041442	.831915	-1.993765
15	1	0	-.131482	-1.447585	1.316523
16	1	0	2.405374	.113752	1.445376
17	1	0	-1.802226	1.730213	-1.102170
18	1	0	-.301305	.750650	2.376269
19	1	0	2.297314	-1.622811	1.050328
20	1	0	2.439161	-.933716	-1.358228
21	1	0	1.956380	.724387	-.915767

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.945042	.621232	.093454
2	6	0	-1.780526	-.896084	-.081857
3	6	0	-.416152	-1.364012	.415397
4	6	0	-.643176	1.463312	-.024639
5	6	0	.611271	-.731562	-.502635
6	7	0	.555883	.755838	-.499302
7	6	0	2.064349	-.651552	-.001111
8	6	0	1.750812	.808936	.367469
9	1	0	-2.684846	.984845	-.626549
10	1	0	-2.597799	-1.412508	.433735
11	1	0	-1.863026	-1.163655	-1.142929
12	1	0	-.251877	-1.045343	1.454273
13	1	0	-.828198	2.318516	-.685871
14	1	0	-.417510	1.887750	.964876
15	1	0	.484088	-1.151447	-1.511903
16	1	0	2.338666	-1.323647	.816380
17	1	0	-2.372110	.807868	1.084840
18	1	0	-.331482	-2.457604	.388870
19	1	0	2.794551	-.743014	-.807943
20	1	0	2.483679	1.577496	.094668
21	1	0	1.505467	.928254	1.436212

Rotational constants (GHZ): 3.5902640 1.9706760 1.4377411

Isotopes: C-12,C-12,C-12,C-12,C-12,N-14,C-12,C-12,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1

Dipole moment (Debye):

X= -.3049 Y= -.6619 Z= 1.0322 Tot= 1.2635

Quadrupole moment (Debye-Ang):

XX= -50.0778 YY= -51.1425 ZZ= -52.0497

XY= -.7995 XZ= .8120 YZ= 1.4939

Octapole moment (Debye-Ang**2):

XXX= 3.5896 YYY= .8391 ZZZ= 1.2109 XXY= -.1115

XXY= 1.1945 XXZ= -.8096 XZZ= -1.0879 YZZ= -1.4572

YYZ= .3215 XYZ= 1.5546

Hexadecapole moment (Debye-Ang**3):

XXXX= -740.9862 YYYY= -406.4822 ZZZZ= -134.9972 XXXY= 3.3580

XXXZ= -5.1263 YYYY= .1759 YYYZ= -1.5894 ZZZX= 1.0031

ZZZY= 3.9432 XXYY= -190.8317 XXZZ= -143.6864 YYZZ= -91.7996

XXYZ= -1.9706 YYXZ= 1.9592 ZZXY= -3.3395

N-N= 4.043649606073D+02 E-N=-1.570539120879D+03 KE= 3.266343788739D+02

Exact polarizability: 79.345 -4.420 65.464 .536 -.883 74.681

Approx polarizability: 63.193 -.062 63.881 .746 1.351 64.780

Rotating electric field derivatives to standard orientation.

Rotating nuclear coordinate derivatives to standard orientation.

Full mass-weighted force constant matrix:

Low frequencies --- -195.2818 -.0009 -.0001 .0005 .4356 .5779

Low frequencies --- .8345 111.3406 255.2609

***** 1 imaginary frequencies (negative Signs) *****

Harmonic frequencies (cm**1), IR intensities (KM/Mole),

Raman scattering activities (A**4/AMU), Raman depolarization ratios,

reduced masses (AMU), force constants (mDyne/A) and normal coordinates:

		1		2		3			
		?A		?A		?A			
Frequencies --		-195.2818		111.3406		255.2609			
Red. masses --		1.7181		2.0738		1.9147			
Frc consts --		.0386		.0151		.0735			
IR Inten --		.2666		.3811		.1650			
Raman Activ --		.0000		.0000		.0000			
Depolar --		.0000		.0000		.0000			
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	.03	-.01	.16	.00	-.01	.08	.01	.01	.00
2 6	.01	.02	-.03	-.01	.02	-.13	-.05	-.03	.14
3 6	.00	-.02	-.04	-.06	-.04	-.03	.03	-.07	-.14
4 6	-.02	.04	-.16	.01	-.02	.08	.01	.01	-.02
5 6	.01	.00	-.02	.01	-.03	.06	.01	.04	-.09
6 7	.01	-.01	.01	-.03	-.03	-.02	.02	.04	-.03
7 6	.00	.00	.03	.00	.01	.12	-.05	-.02	.13
8 6	-.03	-.01	.06	.06	.10	-.16	.01	.03	-.01
9 1	-.19	.05	.41	-.06	.09	.20	.05	-.05	-.07
10 1	-.01	-.02	-.10	-.07	-.04	-.29	.07	.05	.39
11 1	.02	.13	-.06	.11	.17	-.17	-.32	-.14	.19
12 1	-.01	-.06	-.03	-.14	-.07	-.01	.16	-.25	-.11
13 1	-.11	-.18	-.42	.00	.02	.14	-.02	.02	.00
14 1	.00	.36	-.31	.06	-.09	.10	.02	.00	-.02
15 1	.04	.00	-.02	.10	-.06	.06	.11	.10	-.12
16 1	-.01	-.02	.01	-.10	.16	.27	-.30	.02	.24
17 1	.31	-.15	.30	.10	-.15	.15	-.03	.13	-.04
18 1	-.01	-.02	-.08	-.08	-.04	-.06	.03	-.06	-.34
19 1	.02	.04	.04	.05	-.21	.19	.12	-.17	.30
20 1	-.03	.00	.11	.07	.01	-.41	.06	-.05	-.07
21 1	-.07	-.05	.06	.19	.34	-.16	.00	.16	-.03
		4		5		6			
		?A		?A		?A			
Frequencies --		328.3010		348.0079		455.2009			
Red. masses --		2.4631		2.5042		3.3200			
Frc consts --		.1564		.1787		.4053			
IR Inten --		4.1158		.1435		.4530			
Raman Activ --		.0000		.0000		.0000			
Depolar --		.0000		.0000		.0000			
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	.00	.03	-.08	.02	.11	.02	.11	.04	-.03
2 6	-.04	.00	.02	.00	.10	.04	.25	.03	.00
3 6	-.06	-.15	-.02	-.02	-.11	-.03	.13	-.12	.08
4 6	-.02	.06	-.06	.05	-.02	.02	-.01	.15	.02
5 6	-.02	.00	.10	.06	-.13	.03	-.09	.00	-.01
6 7	-.02	-.03	.20	-.05	-.10	-.10	-.13	.01	.03

S77

7	6	.06	.04	-.08	.09	.11	.01	-.16	-.06	.00
8	6	.11	.05	-.03	-.16	.03	.01	-.11	-.03	-.04
9	1	.05	-.03	-.16	.06	.09	-.03	.14	-.12	-.14
10	1	-.06	.08	.07	-.01	.13	.04	.09	.03	-.26
11	1	-.10	-.05	.04	-.05	.14	.03	.47	.12	-.05
12	1	-.07	-.41	.06	.02	-.31	.02	.23	-.25	.10
13	1	.03	-.07	-.24	.13	.08	.13	.00	.14	-.01
14	1	-.14	.26	-.11	.16	-.16	.06	.00	.16	.01
15	1	-.04	.10	.06	.15	-.19	.04	-.16	.02	-.01
16	1	.22	.05	-.13	.29	.15	-.02	-.33	-.06	.06
17	1	-.09	.10	-.13	-.01	.17	.00	-.04	.03	-.09
18	1	-.13	-.16	-.29	-.20	-.12	-.20	.10	-.12	-.10
19	1	-.08	.06	-.21	.04	.27	-.05	-.06	-.15	.10
20	1	.04	.05	-.23	-.25	.18	.18	-.08	-.08	-.09
21	1	.35	.10	.03	-.34	-.08	-.02	-.06	.02	-.03
7					8			9		
?A					?A			?A		
Frequencies --					471.8424			593.6529		
Red. masses --					3.6851			2.4074		
Frc consts --					.4834			.4999		
IR Inten --					1.7634			4.8955		
Raman Activ --					.0000			.0000		
Depolar --					.0000			.0000		
Atom AN		X	Y	Z	X	Y	Z	X	Y	Z
1	6	.21	-.10	-.02	.17	-.01	-.03	.01	.01	-.02
2	6	-.07	-.15	-.02	-.03	-.06	-.04	-.02	-.08	-.06
3	6	-.13	-.10	.07	-.01	.04	-.05	-.01	-.04	-.02
4	6	.14	.04	-.01	.10	.01	.02	-.08	.25	.07
5	6	-.13	.09	.12	-.03	-.05	-.09	.07	-.06	.06
6	7	.09	.13	-.14	-.07	-.11	.15	-.07	.08	-.04
7	6	-.10	.06	-.02	-.04	.06	-.01	.15	-.06	.01
8	6	-.01	.05	.02	-.09	.06	-.01	-.02	-.10	-.08
9	1	.15	-.01	.09	.13	.11	.07	-.08	.03	.09
10	1	-.16	.04	.01	.02	.12	.22	.07	.08	.26
11	1	-.08	-.21	.00	-.26	-.22	.02	-.30	-.28	.02
12	1	-.29	-.27	.15	-.01	.48	-.18	-.17	.14	-.05
13	1	.02	.11	.11	.15	-.01	-.03	-.09	.21	.03
14	1	.15	-.07	.03	.08	.07	.01	-.07	.25	.06
15	1	-.17	.03	.15	.01	.03	-.14	.14	-.07	.06
16	1	.07	.03	-.10	-.08	.07	.01	.12	.11	.17
17	1	.31	-.14	.03	.24	-.11	.02	.04	-.19	.03
18	1	.08	-.08	-.14	.04	.03	.41	.03	-.04	.19
19	1	-.25	.12	-.16	.03	.09	.06	.16	-.24	.05
20	1	.06	.05	.21	-.17	.08	-.15	-.05	.02	.15
21	1	-.21	-.04	-.02	.03	.15	.02	-.06	-.36	-.05
10					11			12		
?A					?A			?A		
Frequencies --					789.4637			794.4961		
Red. masses --					1.3361			1.5178		
Frc consts --					.4906			.5645		
IR Inten --					1.0859			1.0108		
Raman Activ --					.0000			.0000		
Depolar --					.0000			.0000		
Atom AN		X	Y	Z	X	Y	Z	X	Y	Z
1	6	.01	-.01	.07	-.02	.01	.04	.08	-.05	.06
2	6	-.06	-.04	.03	.00	-.03	.00	.04	.02	-.01
3	6	-.05	-.05	.02	.00	-.05	-.03	.00	.13	-.10
4	6	.04	.01	.03	-.02	.09	.03	.01	-.05	.05
5	6	-.01	-.01	-.07	.02	-.10	-.03	.01	.06	.12
6	7	.03	.02	.00	.02	.03	-.06	-.05	-.02	.00
7	6	.05	.03	-.02	-.07	.01	.05	-.01	-.05	.04
8	6	.00	.01	-.02	.04	.00	.06	-.06	-.04	-.06
9	1	.31	-.09	-.27	.08	-.06	-.10	.35	-.09	-.24
10	1	-.19	-.14	-.28	.00	-.06	-.03	.18	-.06	.12
11	1	.14	.23	-.06	-.03	.05	-.02	-.12	.06	-.01
12	1	-.01	.11	-.03	.03	.19	-.11	-.16	-.02	-.03
13	1	-.10	-.16	-.15	-.08	.03	-.02	-.16	-.27	-.19
14	1	.10	.26	-.09	.03	.15	-.01	.07	.29	-.11
15	1	-.03	.05	-.09	.15	-.13	-.04	.09	-.01	.14
16	1	-.14	.15	.14	.25	-.20	-.23	.24	-.06	-.06
17	1	-.34	.23	-.12	-.19	.06	-.04	-.27	.08	-.12

S78

18	1	.01	-.05	.19	.00	-.06	.24	.08	.15	-.27
19	1	.19	-.15	.13	-.21	.42	-.12	-.24	.02	-.18
20	1	-.07	.13	.12	.23	-.27	-.19	-.06	-.04	-.06
21	1	-.03	-.17	.00	.07	.38	.01	-.10	-.01	-.07

13

14

15

?A

?A

?A

Frequencies -- 890.0798 927.2330 984.2653

Red. masses -- 2.6861 1.8947 1.5554

Frc consts -- 1.2538 .9598 .8878

IR Inten -- 2.6768 1.3367 2.1305

Raman Activ -- .0000 .0000 .0000

Depolar -- .0000 .0000 .0000

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	.17	-.12	-.03	.06	-.02	-.03	.03	-.06	.00
2	6	.09	.17	.04	-.08	-.02	.04	.01	-.01	.09
3	6	-.13	.00	.01	-.03	.03	.06	-.05	.04	-.09
4	6	-.15	-.08	.03	-.01	.01	-.01	.01	.06	-.09
5	6	.01	-.08	-.07	.01	.09	-.07	-.04	-.01	.01
6	7	-.01	.08	-.02	-.05	.02	.01	-.02	.00	.05
7	6	.02	.03	-.01	.15	-.06	.05	-.01	.03	.06
8	6	.06	.00	.03	-.09	-.08	-.02	.02	-.05	-.04
9	1	.13	-.23	-.04	.02	.01	.03	-.09	-.31	.00
10	1	.01	.39	.13	-.27	.02	-.22	-.08	-.17	-.20
11	1	-.02	.04	.08	.20	.04	.00	.21	.27	.00
12	1	-.05	.03	-.01	.09	-.16	.10	.13	.15	-.15
13	1	-.35	-.13	.02	-.03	.05	.04	.09	.29	.19
14	1	-.23	-.01	.01	-.03	-.02	.02	-.07	-.30	.09
15	1	.01	-.04	-.08	-.10	.12	-.07	.18	.04	-.04
16	1	-.06	.06	.04	.18	-.23	-.10	.30	.24	.12
17	1	.10	-.16	-.06	.13	.00	-.01	.13	.16	.00
18	1	-.52	-.03	.11	.03	.04	-.16	-.02	.04	.03
19	1	.13	.00	.09	.30	.36	.13	-.22	-.05	-.13
20	1	.10	-.04	.04	-.01	-.27	-.32	.03	-.02	.08
21	1	.11	-.04	.05	-.03	.35	-.05	.05	-.22	-.01

16

17

18

?A

?A

?A

Frequencies -- 985.6748 1001.8715 1024.9581

Red. masses -- 1.9487 2.2377 1.5795

Frc consts -- 1.1155 1.3234 .9777

IR Inten -- .8512 2.4343 3.2390

Raman Activ -- .0000 .0000 .0000

Depolar -- .0000 .0000 .0000

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-.08	-.07	-.02	.01	.06	-.03	.03	-.01	-.08
2	6	.05	-.03	.02	-.04	.01	-.04	-.11	.01	.04
3	6	-.07	.13	.02	.08	-.03	.03	.05	.03	.02
4	6	.09	.10	.06	-.02	-.09	.03	-.01	-.01	.07
5	6	-.04	-.08	-.07	-.04	.03	.00	.06	-.06	-.01
6	7	.05	-.04	.01	-.05	.01	-.01	.01	.04	.02
7	6	-.02	.08	.00	-.05	.18	.05	-.06	-.06	.01
8	6	.00	-.03	-.01	.06	-.19	-.04	-.01	.06	-.03
9	1	-.09	.00	.03	.05	.26	.04	-.01	.22	.09
10	1	.18	-.21	.04	-.10	.13	.00	-.29	.06	-.20
11	1	.22	-.27	.06	-.06	-.07	-.01	.22	-.06	.02
12	1	.08	-.26	.10	.14	-.02	.02	.48	-.08	-.02
13	1	.09	-.03	-.10	-.07	-.21	-.11	-.10	-.17	-.10
14	1	.10	.25	.00	.00	.11	-.06	-.09	.21	.00
15	1	-.12	-.14	-.03	.02	-.02	.01	.29	-.08	-.03
16	1	-.01	.18	.08	.10	.44	.20	.12	-.04	-.03
17	1	-.09	-.28	.01	.06	-.02	.00	.16	-.14	.00
18	1	-.42	.11	-.37	.25	-.02	-.01	-.01	.02	-.10
19	1	.10	.13	.11	-.01	.23	.09	-.29	-.17	-.18
20	1	.03	-.06	-.01	.27	-.38	.02	-.06	.17	.12
21	1	.02	-.03	-.01	.13	-.28	-.03	-.08	-.08	-.03

19

20

21

?A

?A

?A

Frequencies -- 1063.3102 1094.1771 1135.2103

Red. masses -- 2.0399 3.2615 2.0169

Frc consts -- 1.3589 2.3006 1.5314

IR Inten -- 3.5889 16.2327 8.9085

Raman Activ -- .0000 .0000 .0000

S79

Depolar	--	.0000			.0000			.0000		
Atom AN		X	Y	Z	X	Y	Z	X	Y	Z
1	6	-.09	.01	-.03	-.07	-.05	-.01	-.01	-.12	.03
2	6	.09	.05	.00	.00	.03	.02	-.08	.11	-.07
3	6	-.02	-.10	-.01	-.02	-.05	.03	.11	.02	.02
4	6	.04	-.05	.04	.12	-.05	-.04	.01	.06	-.03
5	6	-.12	.04	-.03	.20	-.01	.06	-.05	-.10	.02
6	7	.10	.05	.02	.06	.18	.11	.12	.02	.04
7	6	.06	-.07	.09	-.09	.03	-.08	-.01	-.01	-.02
8	6	-.05	.01	-.08	-.18	-.09	-.11	-.07	.00	-.01
9	1	-.14	.04	.05	-.08	-.02	.02	.00	-.28	-.07
10	1	.11	.12	.09	.14	-.16	.05	-.13	.30	.05
11	1	.01	-.10	.04	-.06	.12	.00	-.36	.22	-.07
12	1	.12	.19	-.12	-.26	-.01	.06	.12	-.07	.05
13	1	.05	-.18	-.12	.07	-.03	-.01	-.04	.12	.07
14	1	-.04	.13	-.02	-.07	-.05	.01	-.09	-.09	.06
15	1	-.22	.39	-.16	.40	.07	.02	-.32	-.16	.08
16	1	.47	.10	.09	-.31	-.01	-.06	.09	.20	.12
17	1	-.03	-.15	.03	.06	.11	.02	-.16	-.09	-.04
18	1	-.10	-.11	.27	-.35	-.08	.22	.40	.04	-.15
19	1	-.13	.06	-.10	.03	.07	.04	.07	.02	.05
20	1	-.07	.08	.05	.06	-.35	-.19	-.12	-.01	-.15
21	1	-.24	.03	-.13	-.05	.03	-.09	.09	.07	.03

22

23

24

?A

?A

?A

Frequencies --	1149.1867	1182.9074	1192.4723
Red. masses --	1.8455	1.3007	1.9138
Frc consts --	1.4360	1.0723	1.6034
IR Inten --	9.7575	1.9079	3.5792
Raman Activ --	.0000	.0000	.0000
Depolar --	.0000	.0000	.0000

Atom AN		X	Y	Z	X	Y	Z	X	Y	Z
1	6	-.05	-.11	-.01	.03	.02	.01	.01	.02	.13
2	6	-.02	.09	.01	-.01	-.02	-.01	.00	-.03	-.11
3	6	.00	-.04	.02	.02	.03	.01	-.01	.01	.12
4	6	.05	.07	.03	-.04	-.01	-.01	-.03	.00	-.10
5	6	.05	.12	.00	.00	-.06	-.02	.04	.04	-.12
6	7	-.04	-.12	-.01	.00	.00	.07	.00	.01	.06
7	6	-.02	.04	.01	-.01	-.02	.00	-.03	-.02	.07
8	6	.06	-.01	-.04	.03	.06	-.08	.01	.01	-.05
9	1	-.14	-.33	-.03	.04	.03	.01	.27	.07	-.12
10	1	-.23	.38	-.02	.08	-.15	.01	-.03	.23	.11
11	1	-.07	.05	.03	-.07	.10	-.04	-.06	-.39	-.01
12	1	.02	.06	-.01	-.10	-.06	.05	.07	-.19	.16
13	1	.19	.01	-.08	-.02	.02	.01	-.06	.20	.16
14	1	.10	.11	.01	-.18	-.03	.04	.14	-.27	-.03
15	1	.23	.11	-.02	-.22	-.07	.01	.24	.02	-.13
16	1	-.22	-.24	-.16	.01	-.04	-.02	.20	-.01	-.01
17	1	-.14	-.29	-.01	.08	.17	.00	-.33	-.03	-.01
18	1	.05	-.04	.10	.03	.03	-.07	-.21	.00	-.08
19	1	-.02	.10	.01	.12	.14	.09	-.22	.01	-.11
20	1	.19	-.03	.23	.45	-.14	.43	-.03	.09	.07
21	1	-.31	-.04	-.13	-.53	.08	-.21	.02	-.16	-.02

25

26

27

?A

?A

?A

Frequencies --	1204.7998	1239.4154	1263.3272
Red. masses --	2.1528	1.4280	1.7799
Frc consts --	1.8411	1.2924	1.6737
IR Inten --	14.0771	1.4581	15.4565
Raman Activ --	.0000	.0000	.0000
Depolar --	.0000	.0000	.0000

Atom AN		X	Y	Z	X	Y	Z	X	Y	Z
1	6	.03	.09	-.02	-.01	-.04	-.04	.05	.02	.03
2	6	.07	-.06	.05	-.02	.03	-.01	-.04	-.01	-.01
3	6	-.08	.01	.01	.05	-.01	.03	.01	.00	-.05
4	6	-.12	.01	.08	.05	.00	.01	-.10	.03	-.01
5	6	.05	.03	-.08	-.01	-.02	-.05	.00	.00	.12
6	7	.16	-.06	.02	-.05	.04	.00	.12	-.07	-.01
7	6	-.06	.01	.02	-.01	.01	.11	.00	.07	.03
8	6	-.04	-.02	-.06	.06	.00	-.06	-.02	-.04	-.07
9	1	-.18	-.19	.05	-.05	.02	.03	.16	.15	-.02

S80

10	1	-.17	.21	-.06	.15	-.20	.04	.03	-.12	-.01
11	1	.08	.02	.03	-.19	.27	-.05	.09	-.11	.00
12	1	-.50	-.05	.09	-.20	-.07	.09	.41	.09	-.13
13	1	.12	-.07	-.08	-.05	-.04	-.02	-.05	.08	.05
14	1	-.19	.08	.05	-.03	.05	.00	-.15	-.11	.05
15	1	.17	-.23	.00	-.13	-.11	.00	-.20	.34	.01
16	1	.00	-.01	-.02	-.03	-.37	-.20	-.34	-.31	-.18
17	1	.09	.05	.02	.15	.14	.00	-.08	-.05	-.01
18	1	.44	.05	-.10	-.06	-.02	.02	-.27	-.02	.08
19	1	-.07	.14	-.01	-.03	.30	.06	.05	.21	.07
20	1	-.21	.12	-.10	-.27	.34	.01	-.14	.07	-.06
21	1	.06	-.13	-.03	.21	-.37	.01	.03	-.16	-.05
28 29 30										
?A ?A ?A										
Frequencies -- 1284.5617 1301.5574 1311.6476										
Red. masses -- 1.6096 1.5077 1.3088										
Frc consts -- 1.5649 1.5048 1.3266										
IR Inten -- 7.1010 6.9925 3.5595										
Raman Activ -- .0000 .0000 .0000										
Depolar -- .0000 .0000 .0000										
Atom AN		X	Y	Z	X	Y	Z	X	Y	Z
1	6	-.03	.04	.04	.00	.00	-.01	.01	.03	.04
2	6	.05	.00	.00	.01	.00	-.01	.00	-.04	-.02
3	6	-.08	.00	-.06	.01	.00	.02	.00	.04	.00
4	6	.07	-.05	-.04	.00	.00	.01	.02	-.03	.01
5	6	-.08	-.06	.05	-.04	-.02	-.05	.06	-.07	.01
6	7	-.03	.10	.04	.02	.01	.01	-.06	.03	-.05
7	6	.05	.02	.01	.12	.13	.06	-.01	.00	.03
8	6	.01	.01	-.04	-.04	-.03	.01	-.03	.05	.00
9	1	-.02	-.07	-.03	-.02	-.01	.01	-.08	-.28	-.02
10	1	-.12	.25	-.02	.04	-.02	.02	-.15	.19	-.03
11	1	.20	-.30	.07	-.08	.07	-.02	.00	-.09	-.01
12	1	.24	.12	-.15	-.04	-.04	.04	.01	-.05	.02
13	1	-.03	-.02	.02	-.03	-.01	.00	.52	-.08	-.18
14	1	-.01	-.06	-.02	-.05	.02	.01	-.29	.03	.06
15	1	.14	-.39	.15	-.06	-.11	-.02	-.30	.37	-.12
16	1	-.21	-.31	-.17	-.25	-.30	-.17	.03	-.05	-.03
17	1	-.12	-.08	.02	.05	.08	.00	-.04	.09	.01
18	1	.38	.04	-.10	.01	.00	-.03	-.01	.04	-.05
19	1	.19	.14	.12	-.41	-.61	-.33	-.06	-.02	-.02
20	1	-.01	.06	.07	.11	-.19	-.03	.16	-.12	.03
21	1	.01	-.10	-.03	-.07	.14	-.02	.25	-.20	.09
31 32 33										
?A ?A ?A										
Frequencies -- 1317.8215 1335.5244 1364.7916										
Red. masses -- 1.1711 1.1579 1.4543										
Frc consts -- 1.1983 1.2169 1.5960										
IR Inten -- .4215 .7078 7.7080										
Raman Activ -- .0000 .0000 .0000										
Depolar -- .0000 .0000 .0000										
Atom AN		X	Y	Z	X	Y	Z	X	Y	Z
1	6	.02	.00	.04	.00	-.03	.00	-.01	.02	.01
2	6	-.01	.00	-.03	-.01	.04	.08	.00	-.02	.03
3	6	.01	-.01	.02	.00	-.02	-.03	.06	.02	-.05
4	6	-.01	-.01	.01	-.01	.01	-.05	.03	-.01	-.03
5	6	-.05	.04	-.01	.01	-.01	-.02	.05	-.05	.01
6	7	.00	.02	-.02	-.01	.01	.00	-.03	.04	.02
7	6	.00	.00	-.02	.01	.00	.01	-.03	.03	.01
8	6	.04	-.05	.02	-.02	.02	.00	.09	-.10	.02
9	1	.08	.00	-.02	.28	.49	-.02	-.01	-.01	.00
10	1	.10	-.10	.05	.03	-.11	-.03	-.25	.22	-.11
11	1	-.10	.06	-.04	.12	.10	.06	.17	-.17	.05
12	1	.18	-.01	.00	-.29	.02	.01	-.35	.00	.02
13	1	.51	-.03	-.16	.23	.07	-.03	-.13	.03	.06
14	1	-.52	.01	.12	-.18	-.10	.04	-.06	.00	.00
15	1	.27	-.26	.07	-.10	-.04	.01	-.32	.15	-.03
16	1	.01	.06	.03	.02	-.02	-.01	-.04	.05	.02
17	1	-.04	.03	.00	-.25	-.54	-.01	-.07	-.06	.01
18	1	-.15	-.02	.02	.19	-.01	.04	-.10	.01	.01
19	1	.05	-.01	.02	-.04	-.03	-.02	-.10	-.04	-.05
20	1	-.21	.15	-.08	.09	-.07	.02	-.35	.28	-.09

S81

```

21 1  -.20  .20  -.07  .09  -.09  .03  -.37  .31  -.14
      34      35      36
      ?A      ?A      ?A
Frequencies -- 1376.5448      1411.0517      1414.4290
Red. masses -- 1.3210      1.4000      1.3691
Frc consts -- 1.4748      1.6423      1.6137
IR Inten -- 4.9401      .6689      3.3810
Raman Activ -- .0000      .0000      .0000
Depolar -- .0000      .0000      .0000
Atom AN  X   Y   Z   X   Y   Z   X   Y   Z
 1 6  -.01  -.02  .01  .08  .14  -.01  .00  .03  -.03
 2 6  .01  -.05  .02  -.07  .01  .00  .07  -.10  .02
 3 6  .10  .00  -.06  .04  -.01  .00  -.06  .04  .03
 4 6  -.04  -.01  .01  .02  -.03  -.01  -.04  -.03  -.01
 5 6  -.03  .06  .00  .00  .03  -.01  .03  -.03  .01
 6 7  .02  .01  .01  .00  .01  .01  -.01  .04  .02
 7 6  .01  -.02  .01  .00  -.01  .01  -.01  .01  .00
 8 6  -.03  .03  -.01  -.01  .01  .00  .02  -.03  -.01
 9 1  .03  .07  .00  -.25  -.57  -.03  .01  .10  -.02
10 1  -.28  .27  -.11  .12  -.31  .00  -.09  .14  .01
11 1  .00  -.01  .00  .01  .02  -.01  -.40  .56  -.11
12 1  -.12  .08  -.06  .00  -.03  .01  .31  -.06  .00
13 1  .21  .00  -.04  -.11  -.04  .02  .19  .03  .00
14 1  .21  -.01  -.05  .04  -.02  -.02  .39  .00  -.12
15 1  -.19  -.49  .24  -.08  -.16  .08  -.05  .08  -.02
16 1  .02  .00  .03  .02  .01  .01  -.02  -.02  -.02
17 1  .02  .09  .00  -.25  -.56  -.02  -.07  -.30  .00
18 1  -.53  -.05  .09  -.15  -.03  .08  -.01  .04  -.05
19 1  .01  .03  .00  -.03  .00  -.02  .01  .00  .01
20 1  .11  -.09  .03  .02  -.02  .00  -.09  .09  .01
21 1  .10  -.10  .04  .01  -.03  .00  -.09  .09  -.04
      37      38      39
      ?A      ?A      ?A
Frequencies -- 1437.8194      1449.2784      1543.4399
Red. masses -- 1.4237      1.5044      1.0998
Frc consts -- 1.7341      1.8617      1.5437
IR Inten -- 3.0694      13.6079      4.0663
Raman Activ -- .0000      .0000      .0000
Depolar -- .0000      .0000      .0000
Atom AN  X   Y   Z   X   Y   Z   X   Y   Z
 1 6  .02  -.04  .00  -.02  .01  .00  .01  .00  .00
 2 6  -.04  .08  -.02  .05  -.03  .00  .00  .00  .00
 3 6  -.07  -.04  .00  -.09  -.02  .00  .01  -.05  .06
 4 6  -.08  -.01  .02  .09  .02  -.01  .00  .00  .00
 5 6  .10  .02  -.02  .12  .08  -.03  .01  -.01  .00
 6 7  -.01  .03  .02  -.01  -.04  -.01  .00  .00  .00
 7 6  -.02  .01  .01  -.02  -.01  .01  .03  -.03  .00
 8 6  .02  -.03  .00  .00  .00  .01  .00  -.01  -.01
 9 1  .02  -.07  -.01  .02  .08  -.01  -.04  .01  .05
10 1  .20  -.24  .04  -.03  .06  -.03  .00  -.04  -.03
11 1  .16  -.25  .05  -.16  .08  -.02  -.04  .00  .01
12 1  .18  .04  -.07  .34  .04  -.08  -.07  .59  -.13
13 1  .41  .04  -.07  -.39  -.03  .06  .01  .00  .01
14 1  .44  .02  -.11  -.46  .00  .13  -.01  .01  .00
15 1  -.42  -.21  .12  -.48  -.31  .20  .00  .03  -.02
16 1  .02  .04  .02  .04  .09  .06  -.24  .09  .17
17 1  .09  .14  .00  .00  .01  .02  -.06  .00  -.03
18 1  .22  -.03  .05  .00  -.02  .04  -.09  -.02  -.60
19 1  -.10  -.03  -.05  -.11  .00  -.07  -.16  .21  -.18
20 1  -.08  .06  -.01  .01  -.04  -.06  .00  .05  .13
21 1  -.08  .07  -.03  .00  -.07  .01  .10  .10  .01
      40      41      42
      ?A      ?A      ?A
Frequencies -- 1547.0019      1555.3503      1568.3417
Red. masses -- 1.1069      1.0752      1.0885
Frc consts -- 1.5608      1.5325      1.5774
IR Inten -- 1.8809      2.4402      4.6736
Raman Activ -- .0000      .0000      .0000
Depolar -- .0000      .0000      .0000
Atom AN  X   Y   Z   X   Y   Z   X   Y   Z
 1 6  .00  .00  .00  .05  -.02  -.01  -.04  .01  .01

```

S82

2	6	.00	.00	.01	-.03	-.03	-.02	-.05	-.03	-.03
3	6	.01	-.03	.03	-.01	.00	.00	.00	-.01	.00
4	6	.00	.00	.00	.01	.02	.00	.00	-.03	-.01
5	6	.01	.01	.01	.01	.00	.00	.01	.00	.00
6	7	.01	.00	.00	.00	.00	.00	.00	.00	.00
7	6	-.07	.05	.00	.00	.00	.00	.00	.00	.00
8	6	.00	.00	.01	.00	.00	.00	.00	.01	.01
9	1	-.02	.00	.02	-.31	.14	.40	.19	-.10	-.26
10	1	-.01	-.04	-.05	.11	.17	.37	.13	.21	.47
11	1	-.04	-.02	.01	.35	.23	-.10	.45	.27	-.13
12	1	-.03	.33	-.08	.02	-.01	-.01	-.01	.08	-.02
13	1	-.01	.02	.03	-.04	-.12	-.14	.03	.17	.21
14	1	.00	.02	-.01	.05	-.17	.06	-.06	.26	-.10
15	1	-.03	.00	.02	-.04	-.02	.01	-.03	-.01	.00
16	1	.47	-.17	-.33	.03	-.01	-.02	-.01	.01	.01
17	1	-.02	-.01	-.01	-.43	.18	-.24	.27	-.11	.15
18	1	-.07	-.01	-.32	.00	-.01	.02	-.03	-.01	-.07
19	1	.28	-.41	.34	.01	-.02	.01	-.02	.01	-.01
20	1	-.01	-.05	-.13	.00	.00	.00	.00	-.04	-.10
21	1	-.10	-.10	-.01	.00	.01	.00	-.07	-.09	.00

43

?A

44

?A

45

?A

Frequencies -- 1582.1224 1597.2942 3033.0926

Red. masses -- 1.1006 1.0932 1.0672

Frc consts -- 1.6231 1.6433 5.7846

IR Inten -- 1.3953 4.4366 53.2107

Raman Activ -- .0000 .0000 .0000

Depolar -- .0000 .0000 .0000

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	.03	-.02	-.01	.02	-.01	.00	.00	.00	.00
2	6	.01	.01	.01	.00	.00	.00	.00	.00	.00
3	6	.00	.00	.00	.00	.00	-.01	.00	.00	.00
4	6	-.01	-.04	-.01	.01	-.06	-.01	.00	.00	.00
5	6	-.01	-.01	.00	.00	.01	.00	.00	.00	.00
6	7	.00	.00	.00	.01	-.01	-.01	.00	.00	.00
7	6	.02	-.01	.00	-.01	.01	.00	.00	.00	.00
8	6	.03	.05	.04	-.03	-.04	-.03	.01	-.02	-.07
9	1	-.14	.07	.19	-.11	.05	.15	.00	.00	.00
10	1	-.03	-.06	-.12	-.01	-.01	-.04	.00	.00	.00
11	1	-.12	-.06	.03	-.03	-.03	.01	.00	.00	.00
12	1	.01	-.01	.00	.01	-.07	.01	-.01	-.02	-.05
13	1	.09	.22	.27	.07	.30	.40	.01	-.03	.03
14	1	-.03	.33	-.14	-.14	.47	-.18	-.02	-.01	-.05
15	1	.03	.02	-.02	-.02	-.02	.02	.00	.02	.05
16	1	-.11	.04	.08	.08	-.02	-.06	-.01	.02	-.03
17	1	-.21	.08	-.12	-.17	.06	-.09	.00	.00	.00
18	1	.01	.01	-.01	.00	.00	.08	.00	.02	.00
19	1	-.06	.10	-.08	.04	-.06	.06	.01	.00	-.01
20	1	.01	-.15	-.48	.00	.12	.40	.18	.18	-.10
21	1	-.35	-.39	-.03	.31	.29	.03	-.23	.09	.92

46

?A

47

?A

48

?A

Frequencies -- 3053.0964 3064.5385 3082.2937

Red. masses -- 1.0673 1.0858 1.0621

Frc consts -- 5.8614 6.0078 5.9449

IR Inten -- 52.4665 24.8569 21.4778

Raman Activ -- .0000 .0000 .0000

Depolar -- .0000 .0000 .0000

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	.00	.00	.01	.00	.00	.00	.00	.00	.00
2	6	.00	.00	.00	.00	.00	.00	.00	.00	.01
3	6	.00	.00	.00	.00	.00	.01	-.01	.03	-.06
4	6	-.01	-.05	-.05	.00	.01	.01	.00	.00	.00
5	6	.00	.00	-.01	-.01	-.03	-.08	.00	-.01	-.01
6	7	.00	.00	.00	.00	.00	.00	.00	.00	.00
7	6	.00	.00	.00	.00	.00	.00	.00	.00	.00
8	6	.00	.00	.00	.00	.00	.01	.00	.00	.00
9	1	.02	-.01	.02	.00	.00	.00	.01	.00	.01
10	1	.00	.00	.00	-.01	-.01	.01	.01	.01	-.01
11	1	.00	.00	.01	.00	-.01	-.05	-.01	-.03	-.14
12	1	-.01	-.02	-.06	-.03	-.06	-.18	.12	.24	.74

S83

13	1	-.06	.25	-.23	.01	-.02	.02	-.01	.03	-.03
14	1	.19	.33	.83	-.03	-.05	-.12	.01	.01	.03
15	1	.01	.04	.12	.11	.35	.89	.02	.06	.15
16	1	.00	.00	.00	.00	-.01	.01	.00	.01	-.01
17	1	.04	-.02	-.11	-.01	.00	.02	.00	.00	.00
18	1	.00	.02	.00	.00	.01	.00	.04	-.57	-.03
19	1	.00	.00	-.01	.03	.00	-.04	.01	.00	.00
20	1	.00	-.01	.00	-.01	-.01	.00	.01	.01	-.01
21	1	.00	.00	.05	.02	-.01	-.07	-.01	.00	.04
49 50 51										
?A ?A ?A										
Frequencies -- 3093.5076 3108.4058 3109.6077										
Red. masses -- 1.0624 1.0839 1.0788										
Frc consts -- 5.9900 6.1704 6.1464										
IR Inten -- 26.6957 18.1646 50.4880										
Raman Activ -- .0000 .0000 .0000										
Depolar -- .0000 .0000 .0000										
Atom AN		X	Y	Z	X	Y	Z	X	Y	Z
1	6	.01	.00	.00	-.04	.02	.01	-.04	.02	.03
2	6	-.04	-.04	-.04	.00	.00	-.01	.00	.00	-.01
3	6	.00	.01	.00	.00	.00	.00	.00	.00	.00
4	6	.00	.00	.00	.01	-.03	.06	-.01	.04	-.04
5	6	.00	.00	.00	.00	.00	.00	.00	.00	.00
6	7	.00	.00	.00	.00	.00	.00	.00	.00	.00
7	6	.00	.00	.00	.00	.00	.00	.00	.00	.00
8	6	.00	.00	.00	.00	.00	.00	.00	.00	.00
9	1	-.10	.05	-.10	.33	-.17	.35	.20	-.10	.22
10	1	.40	.25	-.28	.01	.01	-.01	-.06	-.04	.04
11	1	.05	.18	.78	.01	.04	.15	.01	.03	.11
12	1	.00	.01	.00	.00	.00	-.01	.00	.00	.01
13	1	.01	-.03	.02	-.11	.51	-.40	.10	-.49	.39
14	1	.00	.01	.02	-.07	-.12	-.27	.03	.06	.11
15	1	.00	.02	.05	.00	.00	.00	.00	.01	.02
16	1	.00	.00	.00	.00	.00	.00	.00	.00	.01
17	1	-.02	.01	.06	.16	-.07	-.40	.25	-.11	-.62
18	1	.01	-.17	-.01	.00	-.01	.00	.00	-.05	.00
19	1	.00	.00	.00	.00	.00	.00	.00	.00	.00
20	1	.00	.00	.00	.00	.00	.00	.01	.01	-.01
21	1	.00	.00	.00	-.01	.00	.01	.01	.00	-.02
52 53 54										
?A ?A ?A										
Frequencies -- 3128.1346 3139.0494 3140.5716										
Red. masses -- 1.0955 1.0714 1.0931										
Frc consts -- 6.3162 6.2204 6.3523										
IR Inten -- 53.2242 30.6944 35.9715										
Raman Activ -- .0000 .0000 .0000										
Depolar -- .0000 .0000 .0000										
Atom AN		X	Y	Z	X	Y	Z	X	Y	Z
1	6	.00	.00	.00	.00	.00	.00	.00	.00	.00
2	6	.00	.00	.00	-.01	-.01	.01	-.02	-.01	.01
3	6	.00	.01	.00	.00	-.04	-.02	.00	-.07	-.04
4	6	.00	.00	.00	.00	.00	.00	.00	.00	.00
5	6	.00	.00	.00	.00	.00	.00	.00	.00	-.01
6	7	.00	.00	.00	.00	.00	.00	.00	.00	.00
7	6	-.01	.01	.00	-.04	.04	-.01	.02	-.02	.01
8	6	.06	.05	-.04	-.01	-.01	.00	.01	.01	-.01
9	1	.00	.00	.00	.02	-.01	.02	.04	-.02	.04
10	1	-.01	-.01	.01	.12	.08	-.08	.20	.13	-.13
11	1	.00	.00	.00	.00	-.01	-.03	.00	-.01	-.03
12	1	.00	-.01	-.02	.04	.07	.25	.07	.12	.42
13	1	.00	-.01	.01	.00	-.01	.01	.01	-.03	.02
14	1	.00	.00	-.02	.00	.01	.01	.00	.00	.01
15	1	.00	.00	-.01	.00	.01	.01	.01	.04	.10
16	1	.03	-.07	.09	.15	-.40	.50	-.09	.23	-.29
17	1	.00	.00	-.01	.00	.00	-.01	.01	.00	-.03
18	1	.00	-.06	.00	-.03	.37	.01	-.05	.67	.01
19	1	.13	-.01	-.15	.36	-.03	-.41	-.19	.02	.22
20	1	-.62	-.66	.25	.10	.11	-.04	-.10	-.10	.04
21	1	-.05	.04	.23	.00	.00	-.02	-.01	.01	.04
55 56 57										
?A ?A ?A										

S84

Frequencies --	3145.3038	3165.0821	3204.9175
Red. masses --	1.1031	1.1055	1.1097
Frc consts --	6.4294	6.5253	6.7154
IR Inten --	25.8296	45.1920	19.5945
Raman Activ --	.0000	.0000	.0000
Depolar --	.0000	.0000	.0000

Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	-.02	.01	-.03	-.02	.01	-.08	.00	.00	.00
2 6	-.04	-.02	.06	.02	.01	-.03	.00	.00	.00
3 6	.00	.02	.02	.00	.00	-.01	.00	.00	.00
4 6	.00	.01	-.01	.00	.01	-.02	.00	.00	.00
5 6	.00	.00	.00	.00	.00	.00	.00	.00	.00
6 7	.00	.00	.00	.00	.00	.00	.00	.00	.00
7 6	.00	.00	.00	.00	.00	.00	-.03	-.03	.09
8 6	.00	.00	.00	.00	.00	.00	.00	.00	.01
9 1	.26	-.13	.26	.46	-.23	.45	.00	.00	.00
10 1	.53	.33	-.34	-.22	-.14	.14	.00	.00	.00
11 1	-.04	-.11	-.44	.02	.07	.27	.00	.00	.00
12 1	-.04	-.07	-.21	.01	.02	.07	.00	.00	-.01
13 1	.02	-.08	.07	.03	-.12	.09	.00	.00	.00
14 1	.01	.02	.04	.02	.04	.10	.00	.00	.00
15 1	.00	-.02	-.05	.00	.01	.02	-.01	-.01	-.03
16 1	.00	.00	-.01	.00	.00	.00	-.16	.39	-.47
17 1	-.05	.02	.12	-.22	.10	.51	.00	.00	.00
18 1	.01	-.19	.00	.00	.04	.00	.00	.00	.00
19 1	-.01	.00	.01	.00	.00	.00	.51	-.06	-.56
20 1	.00	.00	.00	.00	.00	.00	.04	.05	-.02
21 1	.00	.00	-.01	.00	.00	.00	.01	-.01	-.05

- Thermochemistry -

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Atom 1 has atomic number 6 and mass 12.00000
Atom 2 has atomic number 6 and mass 12.00000
Atom 3 has atomic number 6 and mass 12.00000
Atom 4 has atomic number 6 and mass 12.00000
Atom 5 has atomic number 6 and mass 12.00000
Atom 6 has atomic number 7 and mass 14.00307
Atom 7 has atomic number 6 and mass 12.00000
Atom 8 has atomic number 6 and mass 12.00000
Atom 9 has atomic number 1 and mass 1.00783
Atom 10 has atomic number 1 and mass 1.00783
Atom 11 has atomic number 1 and mass 1.00783
Atom 12 has atomic number 1 and mass 1.00783
Atom 13 has atomic number 1 and mass 1.00783
Atom 14 has atomic number 1 and mass 1.00783
Atom 15 has atomic number 1 and mass 1.00783
Atom 16 has atomic number 1 and mass 1.00783
Atom 17 has atomic number 1 and mass 1.00783
Atom 18 has atomic number 1 and mass 1.00783
Atom 19 has atomic number 1 and mass 1.00783
Atom 20 has atomic number 1 and mass 1.00783
Atom 21 has atomic number 1 and mass 1.00783

Molecular mass: 111.10480 amu.

Principal axes and moments of inertia in atomic units:

	1	2	3
EIGENVALUES --	502.67646	915.79800	1255.26160
X	.99997	-.00663	.00498
Y	.00655	.99986	.01523
Z	-.00508	-.01520	.99987

THIS MOLECULE IS AN ASYMMETRIC TOP.

ROTATIONAL SYMMETRY NUMBER 1.

WARNING-- ASSUMPTION OF CLASSICAL BEHAVIOR FOR ROTATION
MAY CAUSE SIGNIFICANT ERROR

ROTATIONAL TEMPERATURES (KELVIN) .17230 .09458 .06900

ROTATIONAL CONSTANTS (GHZ) 3.59026 1.97068 1.43774

1 IMAGINARY FREQUENCIES IGNORED.

Zero-point vibrational energy 519798.2 (Joules/Mol)

124.23474 (Kcal/Mol)

WARNING-- EXPLICIT CONSIDERATION OF 7 DEGREES OF FREEDOM AS

VIBRATIONS MAY CAUSE SIGNIFICANT ERROR
 VIBRATIONAL TEMPERATURES: 160.19 367.26 472.35 500.70 654.93
 (KELVIN) 678.87 854.13 1032.79 1135.86 1143.10
 1198.48 1280.62 1334.07 1416.13 1418.16
 1441.46 1474.68 1529.86 1574.27 1633.31
 1653.41 1701.93 1715.69 1733.43 1783.23
 1817.64 1848.19 1872.64 1887.16 1896.04
 1921.51 1963.62 1980.53 2030.18 2035.04
 2068.69 2085.18 2220.65 2225.78 2237.79
 2256.48 2276.31 2298.14 4363.92 4392.70
 4409.16 4434.71 4450.84 4472.28 4474.01
 4500.66 4516.37 4518.56 4525.36 4553.82
 4611.13

Zero-point correction= .197981 (Hartree/Particle)
 Thermal correction to Energy= .204308
 Thermal correction to Enthalpy= .205252
 Thermal correction to Gibbs Free Energy= .167477
 Sum of electronic and zero-point Energies= -327.920408
 Sum of electronic and thermal Energies= -327.914081
 Sum of electronic and thermal Enthalpies= -327.913137
 Sum of electronic and thermal Free Energies= -327.950912

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	128.205	25.534	79.505
ELECTRONIC	.000	.000	.000
TRANSLATIONAL	.889	2.981	40.032
ROTATIONAL	.889	2.981	27.849
VIBRATIONAL	126.428	19.572	11.624
VIBRATION 1	.607	1.940	3.245
VIBRATION 2	.666	1.754	1.694
VIBRATION 3	.712	1.619	1.268
VIBRATION 4	.726	1.579	1.175
VIBRATION 5	.814	1.349	.780
VIBRATION 6	.829	1.313	.732
VIBRATION 7	.951	1.045	.461
Q	LOG10(Q)	LN(Q)	
TOTAL BOT	.925557D-77	-77.033597	-177.376412
TOTAL V=0	.107292D+15	14.030568	32.306576
VIB (BOT)	.738895D-90	-90.131417	-207.535258
VIB (BOT) 1	.183899D+01	.264579	.609216
VIB (BOT) 2	.762678D+00	-.117659	-.270919
VIB (BOT) 3	.569728D+00	-.244333	-.562597
VIB (BOT) 4	.530846D+00	-.275031	-.633283
VIB (BOT) 5	.375137D+00	-.425811	-.980465
VIB (BOT) 6	.356927D+00	-.447421	-1.030224
VIB (BOT) 7	.253169D+00	-.596589	-1.373696
VIB (V=0)	.856539D+01	.932747	2.147730
VIB (V=0) 1	.240575D+01	.381250	.877861
VIB (V=0) 2	.141196D+01	.149824	.344982
VIB (V=0) 3	.125802D+01	.099686	.229537
VIB (V=0) 4	.122924D+01	.089638	.206400
VIB (V=0) 5	.112508D+01	.051184	.117856
VIB (V=0) 6	.111433D+01	.047012	.108250
VIB (V=0) 7	.106044D+01	.025487	.058685
ELECTRONIC	.100000D+01	.000000	.000000
TRANSLATIONAL	.460320D+08	7.663060	17.644847
ROTATIONAL	.272120D+06	5.434761	12.513999

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr)		
		X	Y	Z
1	6	-.000000290	.000000177	.000000047
2	6	-.000000298	-.000000027	.000000027
3	6	-.000000037	-.000000049	.000000007
4	6	.000000056	.000000074	-.000000017
5	6	.000000086	.000000014	-.000000048
6	7	.000000256	.000000247	-.000000106
7	6	.000000518	-.000000072	.000000024

S86

8	6	.000000334	.000000192	-.000000083
9	1	.000000264	.000000169	.000000113
10	1	.000000212	-.000000331	-.000000180
11	1	.000000217	.000000394	-.000000185
12	1	-.000000100	-.000000099	.000000058
13	1	.000000046	.000000028	.000000063
14	1	-.000000027	-.000000058	.000000029
15	1	.000000053	.000000056	-.000000071
16	1	-.000000358	-.000000513	-.000000515
17	1	-.000000015	-.000000357	.000000165
18	1	.000000008	-.000000020	-.000000021
19	1	-.000000199	.000000816	-.000000156
20	1	-.000000620	.000000471	.000000705
21	1	-.000000107	-.000001111	.000000143

Cartesian Forces: Max .000001111 RMS .000000290
1\1\GINC-ARMON\Freq\RMP2-FC\6-31G(d)\C7H13N1\BELOSTOT\19-Oct-2002\0\#
MP2/6-31G* OPT=(CARTESIAN, NEWTON, TS, CALCALL)\1-Azabicyclo4.2.0octan
e, 5-sofa transition state\0,1\C,-1.7566178219,0.6801252543,-0.793457
4973\C,-1.7414224682,0.6300618275,0.7418954179\C,-0.3152194905,0.68199
34075,1.2813222187\C,-0.5356092859,0.0324274545,-1.5058670074\C,0.3600
000934,-0.595612403,0.8228749501\N,0.3856528651,-0.7399177353,-0.65832
59565\C,1.8988606945,-0.6311546268,0.8258501573\C,1.8084194409,-0.3435
634701,-0.6828885819\H,-2.6808746347,0.2192249678,-1.1557399784\H,-2.3
538424397,1.4474315147,1.138521928\H,-2.2012633087,-0.302515962,1.0927
812516\H,0.2160877432,1.5602906531,0.8887590086\H,-0.8948019023,-0.617
4771459,-2.3129849438\H,0.0414419414,0.8319149773,-1.9937651127\H,-0.1
314822494,-1.4475846971,1.3165230347\H,2.4053742862,0.113751662,1.4453
763757\H,-1.8022261763,1.7302129316,-1.1021695528\H,-0.3013050868,0.75
06503504,2.3762690206\H,2.2973137216,-1.6228111684,1.0503279873\H,2.43
91610509,-0.9337158015,-1.3582279299\H,1.956380025,0.7243872018,-0.915
7673378\Version=IBM-RS6000-G98RevA.7\HF=-327.043992\MP2=-328.118389\R
MSD=9.619e-09\RMSF=2.897e-07\Dipole=-0.0115742,0.4266601,0.1843406\

Conformation 6 (RINI transition state)

Item	Value	Threshold	Converged?
Maximum Force	.000031	.000450	YES
RMS Force	.000008	.000300	YES
Maximum Displacement	.001465	.001800	YES
RMS Displacement	.000501	.001200	YES
Predicted change in Energy	=-1.967847D-08		

Optimization completed.

```
-- Stationary point found.
```

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.693507	.741298	-.719931
2	6	0	-1.702612	.664157	.813393
3	6	0	-.282541	.727521	1.394863
4	6	0	-.872811	-.402686	-1.330843
5	6	0	.509547	-.438098	.821648
6	7	0	.358674	-.511731	-.612468
7	6	0	2.039858	-.332481	.585875
8	6	0	1.768819	-.579203	-.926391
9	1	0	-2.720516	.718526	-1.106362
10	1	0	-2.315734	1.476502	1.220805
11	1	0	-2.178832	-.276034	1.127260
12	1	0	.193723	1.668716	1.089776
13	1	0	-1.464138	-1.337770	-1.292411
14	1	0	-.655540	-.205928	-2.387913
15	1	0	.219284	-1.367462	1.352667
16	1	0	2.436292	.663912	.798592
17	1	0	-1.247398	1.696231	-1.024179
18	1	0	-.304158	.700494	2.492022
19	1	0	2.654589	-1.081345	1.090872
20	1	0	2.129363	-1.554865	-1.294249
21	1	0	2.141826	.198087	-1.611287

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.817273	.699482	.379518
2	6	0	-1.849283	-.754310	-.113006
3	6	0	-.539123	-1.491025	.202364
4	6	0	-.661250	1.479781	-.260950
5	6	0	.595347	-.738290	-.476617
6	7	0	.519611	.676110	-.196242
7	6	0	2.022250	-.712445	.133198
8	6	0	1.889043	.834128	.241136
9	1	0	-2.773064	1.193730	.163240
10	1	0	-2.698163	-1.279565	.340113
11	1	0	-2.016801	-.766352	-1.199767
12	1	0	-.372150	-1.487682	1.287658
13	1	0	-.931098	1.744383	-1.301477
14	1	0	-.483833	2.422024	.271984
15	1	0	.594232	-.983003	-1.558313
16	1	0	2.080124	-1.211647	1.104102
17	1	0	-1.683250	.702014	1.468329
18	1	0	-.585180	-2.536608	-.128677
19	1	0	2.824518	-1.080467	-.510727
20	1	0	2.548051	1.391036	-.446461
21	1	0	2.021066	1.255435	1.249832

Rotational constants (GHZ): 3.5495283 1.9689177 1.4099474

Isotopes: C-12,C-12,C-12,C-12,C-12,N-14,C-12,C-12,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1

Dipole moment (Debye):

X= .0602 Y= -.1496 Z= .2972 Tot= .3381

Quadrupole moment (Debye-Ang):

XX= -50.4067 YY= -50.8752 ZZ= -51.4893

XY= -.4691 XZ= .3915 YZ= .6188

Octapole moment (Debye-Ang**2):

XXX= 3.6107 YYY= 3.2760 ZZZ= 1.1003 XXY= .1178

XXY= .7646 XXZ= -.5200 XZZ= .9039 YZZ= -.4227

YYZ= .6663 XYZ= .9580

Hexadecapole moment (Debye-Ang**3):

XXXX= -753.2425 YYYY= -420.6877 ZZZZ= -128.5945 XXXY= -.3533

XXXZ= -4.1473 YYYY= .2652 YYYZ= 3.9158 ZZZX= 1.9348

ZZZY= .2122 XXYX= -196.1131 XXZZ= -147.3257 YYZZ= -92.9518

XXYZ= -1.1410 YYXZ= .3609 ZZXY= -.4248

N-N= 4.041301507530D+02 E-N=-1.570124511452D+03 KE= 3.266217787192D+02

Exact polarizability: 82.981 -4.329 67.233 -.203 1.612 76.170

Approx polarizability: 64.740 .180 64.298 1.216 1.281 64.868

Rotating electric field derivatives to standard orientation.

Rotating nuclear coordinate derivatives to standard orientation.

Full mass-weighted force constant matrix:

Low frequencies --- -254.2309 -.0006 .0002 .0006 2.2859 3.0694

Low frequencies --- 4.4607 145.2144 196.3549

***** 1 imaginary frequencies (negative Signs) *****

Harmonic frequencies (cm**⁻¹), IR intensities (KM/Mole),

Raman scattering activities (A**4/AMU), Raman depolarization ratios,

reduced masses (AMU), force constants (mDyne/A) and normal coordinates:

1			2			3			
?A			?A			?A			
Frequencies --	-254.2309		145.2143		196.3549				
Red. masses --	3.4780		2.0690		1.9822				
Frc consts --	.1324		.0257		.0450				
IR Inten --	7.3615		1.4388		1.1173				
Raman Activ --	.0000		.0000		.0000				
Depolar --	.0000		.0000		.0000				
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	-.03	.02	-.07	.04	-.04	.10	.06	.04	.07
2 6	.00	.00	-.03	-.01	.02	-.06	-.03	.02	.11
3 6	-.01	-.04	-.05	-.03	-.03	-.08	.01	-.04	-.14
4 6	.01	.00	-.02	-.01	.00	.07	-.02	-.04	-.15
5 6	-.01	.03	.05	.02	-.02	.01	.02	.02	-.06
6 7	-.06	-.05	.37	.00	.00	-.09	-.01	.00	.04
7 6	.02	.01	-.02	-.04	.02	.18	-.02	.01	.05
8 6	.09	.03	-.17	.01	.04	-.14	-.02	.01	.08
9 1	-.03	-.01	-.14	.03	.00	.23	.03	.03	.21
10 1	-.01	.01	-.02	-.03	-.01	-.13	.06	.03	.28
11 1	-.02	-.02	-.03	.02	.14	-.06	-.25	.02	.15
12 1	-.02	-.10	-.05	-.08	-.12	-.07	.08	-.24	-.15
13 1	.17	-.12	-.10	-.10	.10	.12	-.05	-.34	-.22
14 1	-.09	.06	-.09	.05	-.04	.13	-.04	.10	-.41
15 1	.00	.23	.00	.16	-.08	.03	.10	.10	-.08
16 1	-.02	.13	.05	-.24	.24	.30	-.11	-.01	.05
17 1	-.07	.07	-.07	.14	-.16	.09	.26	.10	.05
18 1	-.03	-.02	-.12	-.04	.00	-.16	-.05	.02	-.32
19 1	-.01	-.12	.02	.04	-.19	.39	.04	.02	.12
20 1	-.11	-.12	-.49	.02	-.13	-.28	.00	.02	.11
21 1	.42	.20	-.29	.05	.26	-.24	-.06	-.01	.09

4			5			6			
?A			?A			?A			
Frequencies --	315.6854		372.0283		433.4448				
Red. masses --	1.8404		2.2804		3.2683				
Frc consts --	.1081		.1860		.3618				
IR Inten --	.7204		.1771		1.4190				
Raman Activ --	.0000		.0000		.0000				
Depolar --	.0000		.0000		.0000				
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	.05	.01	.10	.02	-.11	.05	.05	.07	.03
2 6	.03	.09	-.12	-.01	-.05	-.07	.25	.05	.00
3 6	-.06	-.02	.05	.02	.11	.05	.17	-.01	.05
4 6	-.02	-.05	-.06	-.07	-.04	-.06	-.03	.09	-.02
5 6	.00	-.06	.08	-.05	.13	-.01	-.02	-.03	-.13
6 7	-.03	-.05	.03	.05	.12	.02	-.14	-.06	.05

S89

7	6	.07	.04	-.05	-.09	-.08	.00	-.14	-.05	.01
8	6	-.05	.03	.01	.12	-.06	.02	-.15	-.06	.00
9	1	.03	.05	.30	-.01	-.07	.25	-.04	-.10	.01
10	1	-.11	.06	-.41	-.03	-.11	-.18	.16	.02	-.20
11	1	.28	.30	-.16	.11	.02	-.09	.44	.13	-.03
12	1	-.17	-.01	.06	-.01	.32	.05	.33	.16	.02
13	1	-.08	-.24	-.09	-.13	-.29	-.11	-.02	.10	-.02
14	1	.02	.04	-.23	-.23	.10	-.24	.08	.07	-.03
15	1	-.03	-.10	.09	-.12	.15	-.01	-.05	.03	-.14
16	1	.28	.00	-.08	-.22	-.09	.00	-.40	-.04	.03
17	1	.25	-.11	.07	.19	-.21	.03	.06	.12	.02
18	1	-.10	-.02	.05	.19	.05	.22	.09	-.06	.20
19	1	.00	.17	-.20	-.11	-.20	.04	-.01	-.10	.21
20	1	-.10	.12	.03	.17	-.15	.00	-.15	-.09	-.04
21	1	-.08	.00	.03	.21	-.09	.01	-.13	-.03	-.02
7					8			9		
?A					?A			?A		
Frequencies --		454.0159				525.9496			661.2723	
Red. masses --		3.0603				1.7335			2.3229	
Frc consts --		.3717				.2825			.5985	
IR Inten --		.3770				.5793			.2752	
Raman Activ --		.0000				.0000			.0000	
Depolar --		.0000				.0000			.0000	
Atom AN		X	Y	Z	X	Y	Z	X	Y	Z
1	6	-.20	.05	.08	-.10	.04	.03	-.04	.02	-.02
2	6	-.04	.10	.01	.09	.03	.04	.00	.01	-.03
3	6	.05	.17	-.05	.02	-.09	.00	.04	.04	-.04
4	6	-.07	-.16	.05	-.08	.02	.00	-.14	.16	-.05
5	6	.14	-.04	-.12	-.01	.02	.09	.09	-.03	.07
6	7	.01	-.09	.00	.02	.08	-.06	-.09	.03	.00
7	6	.11	-.03	.03	.00	-.04	.00	.12	-.09	.05
8	6	.02	-.03	-.01	.07	-.04	-.01	-.01	-.11	-.01
9	1	-.12	.10	-.16	-.10	-.07	-.26	-.17	-.06	.36
10	1	.04	-.09	-.07	.00	-.03	-.20	.14	-.01	.21
11	1	-.03	.21	.00	.29	.16	.01	-.22	-.12	.01
12	1	.13	.40	-.06	.00	-.48	.01	-.04	.08	-.03
13	1	-.12	-.31	.03	-.15	-.14	-.02	-.09	.32	-.02
14	1	.01	-.07	-.13	-.10	.10	-.15	-.14	.07	.11
15	1	.21	-.03	-.12	-.04	-.01	.09	.24	-.09	.09
16	1	-.02	.00	.05	.07	-.05	-.01	.36	-.20	-.02
17	1	-.42	.11	.11	-.35	.21	.06	.30	-.11	-.06
18	1	-.07	.10	.21	-.03	.04	-.38	.04	.02	.01
19	1	.20	-.02	.14	-.08	-.07	-.08	.02	.07	-.16
20	1	-.01	-.03	-.04	.11	-.08	.00	.03	-.22	-.07
21	1	.02	.01	-.03	.10	-.07	.00	.05	-.02	-.06
10					11			12		
?A					?A			?A		
Frequencies --		778.5984				841.8064			860.5883	
Red. masses --		2.0867				1.4284			1.3778	
Frc consts --		.7453				.5964			.6012	
IR Inten --		.4521				.6103			3.0123	
Raman Activ --		.0000				.0000			.0000	
Depolar --		.0000				.0000			.0000	
Atom AN		X	Y	Z	X	Y	Z	X	Y	Z
1	6	.06	-.04	-.01	.00	.03	.05	-.06	-.02	-.03
2	6	.06	.02	.00	-.06	-.07	.00	-.06	.00	.07
3	6	.04	.15	-.06	-.01	-.09	-.01	.01	.06	.06
4	6	.06	-.11	.03	.04	.06	.00	.02	-.05	-.07
5	6	-.02	.08	.11	-.01	.00	-.07	.00	.04	-.05
6	7	-.01	-.02	-.01	.01	.03	.00	.01	-.03	.00
7	6	-.08	-.05	.05	-.01	.02	.06	.02	-.01	.02
8	6	-.11	.00	-.03	.00	-.01	.04	.00	.00	.02
9	1	.13	.00	-.19	.02	.01	-.11	-.07	.09	.25
10	1	.17	-.03	.14	-.16	-.04	-.16	-.18	-.12	-.29
11	1	-.08	-.01	.02	.05	.09	-.02	.35	.06	.01
12	1	-.04	-.02	-.05	.08	.18	-.03	.18	-.28	.03
13	1	.01	-.13	.04	-.02	-.05	-.02	.18	.30	-.02
14	1	.08	-.10	.00	.08	.12	-.12	.00	-.23	.26
15	1	.06	.02	.12	.06	.04	-.08	-.05	.03	-.05
16	1	.29	-.29	-.10	.18	-.31	-.12	-.03	-.14	-.05
17	1	-.11	-.01	.01	-.14	.12	.07	.28	.02	-.07

S90

18	1	.15	.20	-.23	.09	-.18	.24	-.06	.16	-.26
19	1	-.29	.18	-.35	.01	.40	-.14	.07	.12	.02
20	1	-.08	-.21	-.16	.10	-.37	-.17	.03	-.13	-.07
21	1	-.13	.27	-.14	.04	.37	-.13	-.01	.17	-.05

13

14

15

?A

?A

?A

Frequencies --	879.9903	918.2845	941.4363
Red. masses --	2.2758	2.6444	1.4019
Frc consts --	1.0383	1.3138	.7321
IR Inten --	.4126	1.0894	1.9576
Raman Activ --	.0000	.0000	.0000
Depolar --	.0000	.0000	.0000

Atom AN	X	Y	Z	X	Y	Z	X	Y	Z	
1	6	.11	-.12	-.08	.13	-.05	.00	.03	-.06	.04
2	6	.11	.12	.06	-.07	-.04	.04	-.01	-.03	.08
3	6	-.12	.02	.01	-.05	.03	.02	-.04	.02	-.08
4	6	-.12	-.05	.02	.01	.03	.02	.00	.02	-.08
5	6	-.01	-.05	-.08	-.02	.12	-.01	.02	-.01	.03
6	7	.00	.03	.01	-.05	.06	.00	-.01	.00	.02
7	6	.02	.04	.02	.22	-.08	.02	-.03	-.03	.01
8	6	.06	-.01	.04	-.16	-.11	-.06	.03	.05	-.02
9	1	.07	-.27	-.22	.20	-.04	-.32	.00	-.22	-.19
10	1	.05	.29	.14	-.25	.06	-.18	-.09	-.14	-.21
11	1	.04	.07	.07	.13	.13	.00	.10	.37	.05
12	1	-.05	.04	.00	-.02	-.04	.02	.01	.27	-.09
13	1	-.13	.03	.05	-.07	-.10	.00	.06	.28	-.03
14	1	-.36	-.10	.17	-.11	.10	-.07	-.05	-.12	.19
15	1	-.02	-.02	-.09	-.14	.24	-.04	.25	-.02	.03
16	1	.02	-.12	-.06	.01	.10	.13	.16	.08	.05
17	1	-.01	-.02	-.07	-.16	.14	.03	-.04	.33	.05
18	1	-.47	.01	.07	.13	.05	-.07	.03	-.06	.17
19	1	.11	.25	.02	.41	-.11	.27	-.23	-.19	-.15
20	1	.11	-.22	-.07	-.21	.02	-.01	.01	.22	.11
21	1	.13	.17	-.04	-.18	-.16	-.04	-.05	-.14	.07

16

17

18

?A

?A

?A

Frequencies --	973.6148	980.7647	1037.8217
Red. masses --	2.4858	2.1850	1.4176
Frc consts --	1.3883	1.2383	.8996
IR Inten --	.5568	2.3483	3.4387
Raman Activ --	.0000	.0000	.0000
Depolar --	.0000	.0000	.0000

Atom AN	X	Y	Z	X	Y	Z	X	Y	Z	
1	6	-.05	-.06	.05	.07	.07	-.04	.03	-.02	-.05
2	6	.06	-.06	.02	-.09	.05	-.01	-.06	-.02	.04
3	6	-.06	.12	-.03	.11	-.08	.00	-.01	.05	.03
4	6	.09	.07	-.04	-.07	-.12	.02	.01	.06	.07
5	6	-.08	-.02	.00	.02	.03	.04	.07	-.05	-.05
6	7	-.01	-.04	.00	-.04	.01	-.01	.00	.02	.02
7	6	-.01	.20	.03	-.06	.14	.01	-.06	.00	.02
8	6	.02	-.19	-.02	.02	-.14	-.02	-.02	.00	-.04
9	1	-.13	-.24	.01	.21	.33	-.06	.09	.12	.00
10	1	.18	-.28	-.02	-.18	.17	-.05	-.19	.06	-.13
11	1	.06	-.03	.02	-.06	.14	-.02	.28	-.22	-.01
12	1	-.11	.00	-.03	.16	.05	-.01	.34	-.13	-.03
13	1	.12	.02	-.06	-.07	.05	.07	-.07	-.24	.01
14	1	.24	.08	-.11	-.20	-.21	.21	-.09	.23	-.19
15	1	-.09	-.09	.01	.15	.02	.04	.40	-.12	-.03
16	1	.13	.35	.08	.09	.23	.04	.20	.07	.04
17	1	-.09	-.02	.06	.12	.15	-.05	-.04	-.23	-.04
18	1	-.12	.16	-.14	.32	-.11	.08	-.24	.09	-.09
19	1	.08	.35	.07	-.10	.17	-.05	-.22	-.04	-.16
20	1	.08	-.20	.04	.06	-.15	.02	.01	.10	.07
21	1	.13	-.37	.03	.17	-.35	.04	-.04	-.16	.03

19

20

21

?A

?A

?A

Frequencies --	1074.2839	1100.0909	1113.3676
Red. masses --	1.9119	1.9420	1.8901
Frc consts --	1.3000	1.3847	1.3804
IR Inten --	1.4976	.6198	5.5052
Raman Activ --	.0000	.0000	.0000

S91

Depolar	--	.0000		.0000		.0000				
Atom AN		X	Y	Z	X	Y	Z	X	Y	Z
1	6	.08	-.05	.04	.08	.14	.01	-.04	.04	-.01
2	6	-.09	-.02	-.03	.05	-.15	-.02	.07	-.04	.03
3	6	.04	.07	.05	-.05	.08	-.04	-.09	-.05	-.02
4	6	-.01	.06	-.03	-.09	-.02	.03	.05	-.06	.01
5	6	.15	-.07	.04	-.07	-.06	-.02	.13	.06	.05
6	7	-.02	.00	.02	-.02	-.02	.01	.02	.10	-.02
7	6	-.06	.03	-.11	.03	-.01	.02	-.03	.01	-.06
8	6	-.02	.00	.05	.06	.04	.02	-.11	-.05	.01
9	1	.14	-.04	-.23	.27	.46	-.09	.01	.20	.12
10	1	-.05	-.10	-.04	.20	-.44	-.07	.17	-.27	-.03
11	1	-.15	.16	-.02	.17	-.25	-.04	.12	-.09	.02
12	1	-.27	-.21	.10	-.10	.01	-.03	-.23	.10	.01
13	1	-.09	.07	-.01	-.19	.01	.07	.17	-.04	-.01
14	1	-.05	.06	-.01	-.20	-.03	.08	-.06	-.06	.05
15	1	.09	-.31	.10	-.15	-.13	-.01	.32	.23	.02
16	1	-.49	-.14	-.18	.07	-.01	.02	-.20	-.01	-.07
17	1	-.16	.14	.07	.11	.32	.01	.15	.08	-.03
18	1	.11	.14	-.20	-.07	.10	-.09	-.47	-.11	.23
19	1	.14	.05	.13	.05	.01	.03	.00	-.04	.01
20	1	.01	-.19	-.09	.06	.06	.04	-.21	-.13	-.15
21	1	.13	.11	-.02	.01	.05	.02	.18	-.06	-.02
		22			23			24		
		?A			?A			?A		
Frequencies	--	1149.1934			1166.2117			1193.2054		
Red. masses	--	1.6536			1.2361			1.7013		
Frc consts	--	1.2866			.9905			1.4272		
IR Inten	--	20.8218			3.7825			5.7593		
Raman Activ	--	.0000			.0000			.0000		
Depolar	--	.0000			.0000			.0000		
Atom AN		X	Y	Z	X	Y	Z	X	Y	Z
1	6	.04	.03	.05	-.01	-.01	.02	.00	-.05	.09
2	6	.02	-.04	-.04	.01	.01	-.02	-.03	.04	-.08
3	6	-.07	.00	.05	.00	-.03	.03	.06	-.02	.08
4	6	-.04	-.03	-.06	.01	-.01	-.02	.04	.00	-.10
5	6	.05	.13	-.02	.04	.02	-.01	.00	-.02	-.07
6	7	-.09	-.06	-.01	.01	.02	.06	.01	.06	.02
7	6	.01	.02	.01	-.01	.01	.00	-.03	-.05	.08
8	6	.07	.00	.02	.00	-.02	-.10	-.02	.02	-.03
9	1	.02	-.07	-.10	.05	.10	-.01	.18	.22	-.14
10	1	-.10	.24	.07	.09	-.08	.04	.21	-.19	.09
11	1	.08	-.32	-.04	-.08	.01	-.01	-.21	-.02	-.05
12	1	-.04	-.07	.04	-.13	-.06	.05	.04	-.18	.08
13	1	-.33	.21	.07	.03	.03	-.01	-.07	.21	-.02
14	1	.59	-.17	-.02	-.13	-.02	.06	-.10	-.11	.14
15	1	.26	.14	-.03	.04	.06	-.02	-.13	.11	-.09
16	1	-.05	-.06	-.03	-.05	-.03	-.03	.24	-.08	.05
17	1	-.18	-.10	.07	-.03	.02	.03	-.24	-.07	.11
18	1	-.09	.02	-.02	-.12	-.02	.03	-.31	.02	-.01
19	1	-.12	-.12	-.08	.01	.06	.00	-.01	.18	-.03
20	1	.06	.01	.03	.54	-.11	.32	-.22	.23	-.05
21	1	.03	-.04	.03	-.67	.03	-.04	.27	-.27	.06
		25			26			27		
		?A			?A			?A		
Frequencies	--	1219.1185			1247.8066			1264.1426		
Red. masses	--	1.4284			1.3630			1.5118		
Frc consts	--	1.2508			1.2504			1.4235		
IR Inten	--	2.2682			1.6479			1.3150		
Raman Activ	--	.0000			.0000			.0000		
Depolar	--	.0000			.0000			.0000		
Atom AN		X	Y	Z	X	Y	Z	X	Y	Z
1	6	.00	-.04	.02	.00	.01	.04	.01	-.04	-.05
2	6	-.03	.04	.00	.01	-.01	-.06	-.03	.01	.02
3	6	.04	.00	-.05	.00	.00	.07	.06	-.01	.01
4	6	.02	.02	-.06	.00	-.01	.00	.00	.04	.04
5	6	-.05	-.04	.08	-.01	.03	-.11	.00	.03	-.02
6	7	-.02	.01	-.01	.02	.00	.01	-.05	-.05	-.03
7	6	.04	.02	-.07	.02	.01	-.02	.08	.10	.08
8	6	-.01	-.01	.08	-.03	-.04	.07	.03	-.02	.00
9	1	.17	.24	-.07	-.05	-.10	-.01	.06	.08	-.01

S92

10	1	.07	-.14	-.02	.04	.05	.07	.10	-.25	-.06
11	1	.06	-.09	-.01	-.16	.03	-.03	-.12	.28	.03
12	1	.43	.09	-.11	-.16	-.15	.09	-.13	-.03	.05
13	1	-.18	.12	.01	.21	-.02	-.04	.00	-.11	.00
14	1	.03	-.03	.02	-.18	.00	.04	.04	.11	-.10
15	1	-.08	.16	.05	.17	-.18	-.07	-.21	.10	-.04
16	1	-.01	.28	.06	.28	.41	.17	-.23	-.36	-.14
17	1	-.18	-.25	.04	.03	.20	.03	.09	.03	-.06
18	1	-.26	-.03	.08	.05	.04	-.08	-.26	-.01	.05
19	1	-.03	-.30	.02	-.27	-.40	-.15	-.40	-.39	-.23
20	1	.12	-.29	-.02	-.09	-.17	-.09	-.04	.06	.00
21	1	-.08	.31	-.05	-.06	.30	-.06	.01	-.03	.00

28

29

30

?A

?A

?A

Frequencies -- 1288.9549 1300.2502 1319.3352

Red. masses -- 1.3091 1.4245 1.3320

Frc consts -- 1.2814 1.4190 1.3660

IR Inten -- 5.8666 20.8445 4.1420

Raman Activ -- .0000 .0000 .0000

Depolar -- .0000 .0000 .0000

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-.02	.01	.07	-.02	-.04	-.05	.03	.00	.02
2	6	.03	.01	-.02	.02	.04	.05	-.04	-.01	-.08
3	6	-.05	.00	-.02	.01	-.04	.00	.03	.00	.03
4	6	.03	.01	-.05	.03	.02	.00	-.03	.01	.04
5	6	-.05	.01	.02	-.06	.09	-.02	-.03	.05	.06
6	7	.03	-.01	.00	-.05	-.01	.00	.01	-.03	-.03
7	6	.06	.07	.02	-.01	-.04	-.03	-.02	-.01	-.02
8	6	.00	-.04	-.02	.08	-.04	.02	.06	-.04	.00
9	1	.03	.07	.00	.15	.32	.01	-.10	-.28	-.05
10	1	-.03	.18	.07	.14	-.22	-.02	.05	-.08	.02
11	1	.12	-.29	-.03	-.02	.23	.06	-.17	-.01	-.06
12	1	.17	.06	-.05	-.21	.03	.04	.47	-.04	-.04
13	1	.19	.05	-.07	-.10	-.02	.01	.16	-.07	-.02
14	1	-.45	-.02	.15	.05	.05	-.06	-.01	.04	-.03
15	1	.21	-.25	.07	.38	-.44	.08	.18	.06	.06
16	1	-.32	-.33	-.16	.04	.07	.02	-.07	-.04	-.03
17	1	-.19	-.11	.10	-.04	-.26	-.04	.14	.38	.00
18	1	.19	-.01	-.02	.04	-.05	.04	-.41	.03	.02
19	1	-.09	-.12	-.06	.18	.16	.10	.15	.18	.09
20	1	-.17	.14	-.03	-.22	.23	-.04	-.20	.23	-.02
21	1	-.06	-.01	-.02	-.15	.17	-.04	-.18	.14	-.05

31

32

33

?A

?A

?A

Frequencies -- 1337.0505 1378.4863 1383.1511

Red. masses -- 1.4780 1.2850 1.7278

Frc consts -- 1.5567 1.4386 1.9476

IR Inten -- 7.0383 2.2967 29.2638

Raman Activ -- .0000 .0000 .0000

Depolar -- .0000 .0000 .0000

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-.01	-.02	.00	-.01	-.03	.03	.00	.05	-.03
2	6	.01	.01	-.03	.00	-.04	.01	-.02	.00	.00
3	6	-.02	-.01	.02	.11	.01	-.07	.02	.01	-.02
4	6	.02	-.05	.02	-.03	-.01	.00	.04	-.07	-.02
5	6	-.08	.00	-.02	.01	.03	.01	-.01	-.08	-.02
6	7	-.07	.09	.02	-.02	.03	.01	.05	.15	.08
7	6	.07	-.01	.00	.00	-.01	.01	.02	.04	.01
8	6	-.05	.08	-.02	.01	-.01	.00	.00	-.08	-.02
9	1	.00	-.03	-.03	.08	.13	.00	-.18	-.29	.02
10	1	.09	-.07	.03	-.29	.39	-.01	-.03	-.03	-.05
11	1	-.13	.10	-.01	.12	-.15	-.01	.01	-.04	-.01
12	1	.30	-.02	-.03	-.26	.12	-.01	.00	-.01	-.02
13	1	.17	-.05	-.01	.33	.01	-.08	-.57	.09	.17
14	1	.30	-.06	-.06	.13	-.02	-.02	.24	-.12	.01
15	1	.26	-.46	.09	-.30	-.37	.09	-.12	-.28	.03
16	1	-.08	-.14	-.05	.03	.04	.03	-.08	-.09	-.04
17	1	.13	.15	-.02	-.05	.07	.04	.13	.05	-.05
18	1	-.01	.01	-.02	-.45	-.01	.06	-.02	.00	.01
19	1	.06	-.12	.04	.00	.02	-.01	-.10	-.10	-.05
20	1	.35	-.26	.08	-.02	.02	.00	-.27	.21	-.03

S93

```

21 1 .25 -.24 .08 -.03 .03 -.01 -.27 .16 -.09
      34      35      36
      ?A      ?A      ?A
Frequencies -- 1404.0344      1415.0004      1426.6936
Red. masses -- 1.5207      1.4729      1.5204
Frc consts -- 1.7662      1.7375      1.8234
IR Inten -- 1.9089      1.0745      3.3988
Raman Activ -- .0000      .0000      .0000
Depolar -- .0000      .0000      .0000
Atom AN X Y Z X Y Z X Y Z
1 6 .08 .10 .00 .04 .13 -.02 .05 .02 .01
2 6 -.10 .07 .02 .04 -.13 .00 -.01 .04 .01
3 6 .08 -.02 -.02 .00 .03 .01 -.09 -.01 .00
4 6 .03 -.03 .00 -.02 -.02 -.02 -.06 -.03 .02
5 6 -.03 .04 -.01 .00 .03 .01 .11 -.02 -.01
6 7 -.04 -.02 -.02 .03 -.02 .01 -.07 .07 -.01
7 6 .01 -.02 .00 .00 .00 .00 -.02 .00 .01
8 6 .00 .03 .01 -.02 .01 -.01 .05 -.04 .00
9 1 -.23 -.52 .01 -.10 -.10 .06 .04 -.04 -.07
10 1 .11 -.36 -.09 -.11 .10 -.02 .16 -.26 -.01
11 1 .23 -.30 -.03 -.29 .57 .04 .03 -.02 .00
12 1 -.30 .02 .04 .19 -.07 -.01 .25 -.04 -.05
13 1 .06 -.07 -.01 .02 .06 -.01 .58 .03 -.13
14 1 -.23 -.04 .10 -.14 -.05 .06 .21 -.02 -.08
15 1 .08 -.09 .02 -.04 -.11 .04 -.39 -.10 .00
16 1 .04 .03 .02 -.02 .01 .00 .07 .01 .01
17 1 -.17 -.24 .03 -.23 -.54 .02 -.12 -.25 .03
18 1 -.14 -.04 .07 -.25 .03 .02 .27 -.04 .03
19 1 .03 .01 .01 .01 .01 .00 -.05 -.01 -.01
20 1 .12 -.10 .01 .02 -.05 -.01 -.09 .15 .01
21 1 .09 -.08 .04 .02 -.05 .01 -.12 .13 -.05
      37      38      39
      ?A      ?A      ?A
Frequencies -- 1435.9418      1449.5196      1536.2720
Red. masses -- 3.4439      1.6048      1.1042
Frc consts -- 4.1838      1.9866      1.5354
IR Inten -- 90.3943      40.5508      .6554
Raman Activ -- .0000      .0000      .0000
Depolar -- .0000      .0000      .0000
Atom AN X Y Z X Y Z X Y Z
1 6 .04 -.02 -.02 -.03 -.01 .00 .04 -.01 -.04
2 6 -.04 .08 .01 .02 .01 -.01 .00 .00 .00
3 6 -.02 -.06 -.01 -.06 -.03 -.01 .00 -.05 .04
4 6 -.22 .07 -.01 .11 .02 .00 .00 .00 .00
5 6 .01 .13 .00 .11 .11 .00 .01 -.01 .00
6 7 .29 -.10 .07 -.06 -.05 -.01 .00 .01 .00
7 6 .00 .01 .01 -.02 -.02 .01 -.02 .02 .00
8 6 -.14 .01 -.04 .01 .03 .01 .00 .00 .00
9 1 .08 .05 -.02 -.05 -.04 .01 -.05 .04 .42
10 1 .20 -.35 -.04 .01 -.01 -.05 .00 -.04 -.04
11 1 .08 -.13 .00 -.10 -.08 .00 -.05 .01 .01
12 1 .13 .07 -.03 .29 .06 -.06 .02 .53 .02
13 1 -.06 .12 -.01 -.38 -.13 .08 -.01 -.07 -.02
14 1 .43 -.04 -.04 -.31 .02 .12 .04 -.04 .06
15 1 -.15 -.44 .10 -.49 -.45 .11 -.01 .01 -.01
16 1 -.12 .09 .05 .06 .11 .07 .13 -.08 -.06
17 1 -.08 .00 -.01 .13 .16 -.02 -.38 .17 .02
18 1 -.02 -.08 .06 -.03 -.05 .02 -.06 .14 -.51
19 1 -.11 .07 -.14 -.03 .04 -.04 .04 -.10 .12
20 1 -.04 -.15 -.07 .04 -.11 -.05 -.01 .00 -.01
21 1 .03 -.17 .02 .03 -.10 .05 -.02 .00 .00
      40      41      42
      ?A      ?A      ?A
Frequencies -- 1543.9864      1546.1670      1550.5651
Red. masses -- 1.1088      1.0979      1.0951
Frc consts -- 1.5574      1.5464      1.5512
IR Inten -- 1.5842      8.8045      7.6291
Raman Activ -- .0000      .0000      .0000
Depolar -- .0000      .0000      .0000
Atom AN X Y Z X Y Z X Y Z
1 6 -.03 .02 .04 -.02 .02 .03 -.01 .00 .01

```

S94

2	6	.01	.01	.02	.02	.01	.01	-.05	-.02	-.03
3	6	.01	-.02	.01	.01	-.03	.03	.00	-.02	.01
4	6	-.01	.00	.00	.00	-.01	.00	.01	-.05	.02
5	6	.00	.01	.00	.00	-.02	.00	.01	.01	.00
6	7	.02	-.01	.00	-.01	.01	.00	.00	-.01	.00
7	6	-.05	.05	-.02	.04	-.04	.01	.00	.00	.00
8	6	.00	.01	.00	.00	-.01	.00	.00	.01	.00
9	1	.05	-.05	-.41	.04	-.04	-.30	-.01	-.03	-.07
10	1	-.08	-.03	-.18	-.08	-.03	-.19	.18	.06	.47
11	1	-.15	-.11	.04	-.18	-.09	.04	.44	.24	-.09
12	1	-.03	.18	.01	-.01	.37	.03	.02	.16	.00
13	1	.02	.07	.01	.04	.07	.01	-.01	.42	.12
14	1	-.02	.03	-.05	-.02	.04	-.06	-.14	.22	-.37
15	1	.00	-.01	.01	.03	.05	-.01	-.04	-.04	.01
16	1	.39	-.25	-.18	-.35	.22	.16	.01	.00	.00
17	1	.35	-.21	-.02	.26	-.17	-.01	.08	-.02	-.01
18	1	-.03	.04	-.16	-.04	.10	-.36	-.04	.03	-.15
19	1	.13	-.29	.37	-.12	.26	-.34	.00	.00	.00
20	1	-.04	-.06	-.08	.04	.06	.08	-.01	-.05	-.05
21	1	-.07	-.07	.03	.07	.06	-.03	-.03	-.06	.03

45

?A

Frequencies -- 1560.1906 1608.1755 2964.4604

Red. masses --	1.0953	1.1133	1.0834
----------------	--------	--------	--------

Frc const	--	1.5709	1.6964	5.6097
-----------	----	--------	--------	--------

IR Inten	--	.1403	13.3564	89.5850
----------	----	-------	---------	---------

Raman Activ --	.0000	.0000	.0000
----------------	-------	-------	-------

Depolar	--	.0000	.0000	.0000
---------	----	-------	-------	-------

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	.02	-.01	-.02	.00	.00	.00	.00	.00	.00
2	6	.04	.02	.02	.00	.00	.00	.00	.00	.00
3	6	.00	.01	-.01	.00	.00	.00	.00	.00	.00
4	6	.01	-.06	.02	-.01	.01	.00	.00	.00	.01
5	6	-.01	.00	.00	-.01	-.02	.00	.00	-.01	-.08
6	7	.00	-.01	.00	.00	.02	.00	.00	.00	.00
7	6	.00	.00	.00	.02	-.01	.00	.00	.00	.00
8	6	.00	.01	.00	.06	.06	.02	.00	.00	.00
9	1	-.02	.02	.21	.01	.01	-.01	.00	.00	.00
10	1	-.13	-.05	-.36	.00	.00	-.01	.00	.00	.00
11	1	-.33	-.21	.07	-.01	.00	.00	.00	.00	-.02
12	1	.00	-.13	-.01	-.01	.01	.01	-.01	.00	-.04
13	1	.03	.50	.14	.04	-.08	-.04	-.02	.02	.11
14	1	-.14	.25	-.44	.05	-.04	.07	.00	.02	.01
15	1	.01	-.01	.01	.03	.06	-.02	-.01	.20	.96
16	1	-.01	.00	.00	-.10	.06	.04	.00	.01	-.01
17	1	-.18	.11	.01	.00	-.01	.00	.00	.00	.01
18	1	.02	-.03	.13	.02	.01	-.02	.00	-.03	-.01
19	1	.00	.01	.00	-.03	.07	-.10	.01	-.01	-.02
20	1	-.01	-.05	-.05	-.25	-.34	-.53	.03	.03	-.04
21	1	-.03	-.06	.03	-.50	-.40	.25	.00	.01	.03

48

?A

Frequencies -- 2986.4249 3023.6670 3067.6312

Red. masses --	1.0722	1.0613	1.1044
----------------	--------	--------	--------

Frc consts --	5.6340	5.7167	6.1235
---------------	--------	--------	--------

IR Inten	--	110.3627	138.5225	56.9343
----------	----	----------	----------	---------

Raman Activ --	.0000	.0000	.0000
----------------	-------	-------	-------

Depolar	--	.0000	.0000	.0000
---------	----	-------	-------	-------

[illegible]

S95

13	1	.22	-.21	.92	-.03	.03	-.11	.00	.00	.02
14	1	-.03	-.14	-.10	.00	.01	.00	.00	-.01	.00
15	1	.00	.03	.11	.00	-.02	-.07	.00	.00	.01
16	1	.00	.00	.00	.00	.00	.00	.00	-.02	.06
17	1	.00	.00	-.04	.00	.00	.00	.00	.00	.01
18	1	.00	-.01	.00	.00	.01	.01	.00	-.01	.00
19	1	.00	.00	.00	-.02	.01	.02	-.01	.00	.01
20	1	.06	.05	-.07	.52	.44	-.58	.24	.22	-.25
21	1	.00	.02	.07	.03	.14	.40	-.09	-.34	-.83

49

50

51

?A

?A

?A

Frequencies -- 3079.1833 3082.6910 3089.8314

Red. masses -- 1.0643 1.0598 1.0609

Frc consts -- 5.9452 5.9340 5.9676

IR Inten -- 24.2639 24.2156 26.3863

Raman Activ -- .0000 .0000 .0000

Depolar -- .0000 .0000 .0000

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	.01	.00	.00	.00	.00	.00	-.04	.03	.04
2	6	-.04	-.02	-.05	-.01	.00	.00	.00	.00	-.01
3	6	.00	.00	.01	-.01	.05	-.04	.00	.00	.00
4	6	.00	.00	.00	.00	.00	.00	.00	-.01	-.01
5	6	.00	.00	.00	.00	.00	.00	.00	.00	.00
6	7	.00	.00	.00	.00	.00	.00	.00	.00	.00
7	6	.00	.00	.00	.00	.00	.00	.00	.00	.00
8	6	.00	.00	.00	.00	.00	.00	.00	.00	.00
9	1	-.08	.04	-.02	-.01	.01	.00	.61	-.31	.16
10	1	.35	.22	-.21	.08	.05	-.04	-.06	-.03	.03
11	1	.12	.00	.86	.00	.00	.00	.01	.00	.08
12	1	-.01	.00	-.10	.11	.02	.74	.00	.00	.01
13	1	.00	.00	.01	.00	.00	-.01	.00	-.01	.02
14	1	.00	-.01	.00	.00	.00	.00	.02	.12	.07
15	1	.00	.00	.00	.00	.00	.01	.00	.00	.01
16	1	.00	.00	.00	.00	.01	-.02	.00	.00	.00
17	1	.00	.00	-.04	.00	.00	-.01	-.10	.00	-.68
18	1	-.01	-.04	-.01	-.03	-.61	-.21	.00	.00	.00
19	1	.00	.00	.00	.00	.00	.01	.00	.00	.00
20	1	-.01	-.01	.01	.00	.00	.00	.00	.00	.00
21	1	.00	.00	.01	.00	.01	.01	.00	-.01	-.02

52

53

54

?A

?A

?A

Frequencies -- 3124.5682 3136.1497 3137.6387

Red. masses -- 1.0908 1.0601 1.1002

Frc consts -- 6.2743 6.1430 6.3817

IR Inten -- 32.1233 30.2028 37.6492

Raman Activ -- .0000 .0000 .0000

Depolar -- .0000 .0000 .0000

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	.02	-.01	.00	.00	.00	.00	-.02	.01	-.01
2	6	.00	.00	.00	.00	.00	.00	-.05	-.03	.05
3	6	.00	.00	.00	.00	.00	.00	-.01	-.04	-.03
4	6	-.02	-.07	-.05	.00	.00	.00	.00	.00	.00
5	6	.00	.00	.00	.00	.00	.00	.00	.00	.00
6	7	.00	.00	.00	.00	.00	.00	.00	.00	.00
7	6	.00	.00	.00	-.04	.05	-.02	.00	.00	.00
8	6	.00	.00	.00	.00	.00	.00	.00	.00	.00
9	1	-.18	.09	-.04	.01	-.01	.00	.18	-.09	.04
10	1	.02	.01	-.01	.04	.02	-.02	.58	.36	-.31
11	1	.00	.00	-.02	-.01	.00	-.03	-.05	-.01	-.30
12	1	.00	.00	.00	-.01	.00	-.02	.04	.00	.28
13	1	.03	-.05	.13	.00	.00	.00	.00	.00	.01
14	1	.16	.82	.48	.00	.03	.02	.00	.01	.01
15	1	.00	.00	.00	.00	.00	-.01	.00	.01	.02
16	1	.00	.01	-.02	.02	-.33	.67	.00	.01	-.03
17	1	.00	.00	-.02	.00	.00	.01	.01	.00	.10
18	1	.00	.01	.00	.00	-.04	-.01	.02	.43	.13
19	1	-.02	.01	.01	.47	-.21	-.40	-.01	.00	.00
20	1	.01	.01	-.01	.00	.00	.00	.00	.00	.00
21	1	.00	.00	.00	.00	.01	.03	.00	.00	-.01

55

56

57

?A

?A

?A

S96

Frequencies --	3141.6352	3149.2866	3203.0517
Red. masses --	1.1053	1.1058	1.1098
Frc consts --	6.4277	6.4617	6.7083
IR Inten --	24.0858	55.8887	24.0323
Raman Activ --	.0000	.0000	.0000
Depolar --	.0000	.0000	.0000

Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	.03	-.01	.03	-.05	.02	-.06	.00	.00	.00
2 6	.02	.01	-.03	.02	.01	-.03	.00	.00	.00
3 6	-.01	-.05	-.06	.00	-.01	-.02	.00	.00	.00
4 6	.00	.00	.01	.00	-.01	-.01	.00	.00	.00
5 6	.00	.00	.00	.00	.00	.00	.00	.00	.00
6 7	.00	.00	.00	.00	.00	.00	.00	.00	.00
7 6	.00	.00	.00	.00	.00	.00	-.04	.00	.09
8 6	.00	.00	.00	.00	.00	.00	.00	.00	.01
9 1	-.29	.15	-.06	.47	-.24	.10	.00	.00	.00
10 1	-.26	-.16	.14	-.23	-.15	.12	.00	.00	.00
11 1	.04	.00	.21	.04	.01	.27	.00	.00	.00
12 1	.08	.00	.54	.03	.00	.20	.00	.00	-.02
13 1	-.01	.01	-.03	.01	-.02	.07	.00	.00	.00
14 1	-.01	-.06	-.03	.02	.12	.07	.00	.00	.00
15 1	.00	.01	.04	.00	.00	.02	.00	-.01	-.03
16 1	.00	-.02	.04	.00	.00	.01	-.04	.30	-.57
17 1	-.03	.00	-.27	.08	.01	.66	.00	.00	.00
18 1	.03	.55	.17	.01	.15	.05	.00	-.01	.00
19 1	.05	-.02	-.04	.01	-.01	-.01	.55	-.25	-.45
20 1	.00	.00	.00	.00	.00	.00	.02	.02	-.03
21 1	.00	.00	.00	.00	.00	.00	.00	-.02	-.04

 - Thermochemistry -

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Atom 1 has atomic number 6 and mass 12.00000
 Atom 2 has atomic number 6 and mass 12.00000
 Atom 3 has atomic number 6 and mass 12.00000
 Atom 4 has atomic number 6 and mass 12.00000
 Atom 5 has atomic number 6 and mass 12.00000
 Atom 6 has atomic number 7 and mass 14.00307
 Atom 7 has atomic number 6 and mass 12.00000
 Atom 8 has atomic number 6 and mass 12.00000
 Atom 9 has atomic number 1 and mass 1.00783
 Atom 10 has atomic number 1 and mass 1.00783
 Atom 11 has atomic number 1 and mass 1.00783
 Atom 12 has atomic number 1 and mass 1.00783
 Atom 13 has atomic number 1 and mass 1.00783
 Atom 14 has atomic number 1 and mass 1.00783
 Atom 15 has atomic number 1 and mass 1.00783
 Atom 16 has atomic number 1 and mass 1.00783
 Atom 17 has atomic number 1 and mass 1.00783
 Atom 18 has atomic number 1 and mass 1.00783
 Atom 19 has atomic number 1 and mass 1.00783
 Atom 20 has atomic number 1 and mass 1.00783
 Atom 21 has atomic number 1 and mass 1.00783

Molecular mass: 111.10480 amu.

Principal axes and moments of inertia in atomic units:

	1	2	3
EIGENVALUES --	508.44535	916.61586	1280.00602
X	.99999	-.00278	.00257
Y	.00277	.99999	.00193
Z	-.00258	-.00193	.99999

THIS MOLECULE IS AN ASYMMETRIC TOP.

ROTATIONAL SYMMETRY NUMBER 1.

WARNING-- ASSUMPTION OF CLASSICAL BEHAVIOR FOR ROTATION
 MAY CAUSE SIGNIFICANT ERROR

ROTATIONAL TEMPERATURES (KELVIN) .17035 .09449 .06767

ROTATIONAL CONSTANTS (GHZ) 3.54953 1.96892 1.40995

1 IMAGINARY FREQUENCIES IGNORED.

Zero-point vibrational energy 517470.4 (Joules/Mol)

123.67840 (Kcal/Mol)

WARNING-- EXPLICIT CONSIDERATION OF 7 DEGREES OF FREEDOM AS

VIBRATIONS MAY CAUSE SIGNIFICANT ERROR
 VIBRATIONAL TEMPERATURES: 208.93 282.51 454.20 535.26 623.63
 (KELVIN) 653.22 756.72 951.42 1120.22 1211.16
 1238.19 1266.10 1321.20 1354.51 1400.81
 1411.09 1493.19 1545.65 1582.78 1601.88
 1653.42 1677.91 1716.75 1754.03 1795.31
 1818.81 1854.51 1870.76 1898.22 1923.71
 1983.32 1990.03 2020.08 2035.86 2052.68
 2065.99 2085.52 2210.34 2221.44 2224.58
 2230.90 2244.75 2313.79 4265.17 4296.77
 4350.36 4413.61 4430.23 4435.28 4445.55
 4495.53 4512.19 4514.34 4520.09 4531.09
 4608.45

Zero-point correction= .197094 (Hartree/Particle)
 Thermal correction to Energy= .203529
 Thermal correction to Enthalpy= .204474
 Thermal correction to Gibbs Free Energy= .166575
 Sum of electronic and zero-point Energies= -327.921691
 Sum of electronic and thermal Energies= -327.915256
 Sum of electronic and thermal Enthalpies= -327.914312
 Sum of electronic and thermal Free Energies= -327.952211

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	127.717	25.870	79.765
ELECTRONIC	.000	.000	.000
TRANSLATIONAL	.889	2.981	40.032
ROTATIONAL	.889	2.981	27.880
VIBRATIONAL	125.939	19.909	11.852
VIBRATION 1	.617	1.908	2.734
VIBRATION 2	.636	1.845	2.167
VIBRATION 3	.703	1.644	1.332
VIBRATION 4	.744	1.530	1.071
VIBRATION 5	.794	1.397	.847
VIBRATION 6	.812	1.352	.784
VIBRATION 7	.881	1.193	.596
Q	LOG10(Q)	LN(Q)	
TOTAL BOT	.240671D-76	-76.618575	-176.420789
TOTAL V=0	.109091D+15	14.037788	32.323202
VIB (BOT)	.189101D-89	-89.723306	-206.595547
VIB (BOT) 1	.139825D+01	.145585	.335221
VIB (BOT) 2	.101689D+01	.007275	.016752
VIB (BOT) 3	.597005D+00	-.224022	-.515830
VIB (BOT) 4	.488693D+00	-.310964	-.716021
VIB (BOT) 5	.400906D+00	-.396957	-.914028
VIB (BOT) 6	.376481D+00	-.424257	-.976888
VIB (BOT) 7	.305224D+00	-.515381	-1.186708
VIB (V=0)	.857151D+01	.933057	2.148444
VIB (V=0) 1	.198496D+01	.297751	.685598
VIB (V=0) 2	.163317D+01	.213031	.490522
VIB (V=0) 3	.127873D+01	.106778	.245865
VIB (V=0) 4	.119916D+01	.078876	.181619
VIB (V=0) 5	.114088D+01	.057239	.131799
VIB (V=0) 6	.112589D+01	.051496	.118573
VIB (V=0) 7	.108580D+01	.035750	.082317
ELECTRONIC	.100000D+01	.000000	.000000
TRANSLATIONAL	.460320D+08	7.663060	17.644847
ROTATIONAL	.276485D+06	5.441671	12.529911

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr)		
		X	Y	Z
1	6	-.000001619	.000003340	.000001775
2	6	-.000005550	-.000000496	.000000057
3	6	.000000157	-.000000890	.000001039
4	6	.000004458	-.000004006	-.000003015
5	6	.000003243	.000000986	-.000000993
6	7	-.000010248	-.000004090	-.000002053
7	6	.000019197	.000004052	.000004825

S98

8	6	.000012796	.000000774	.000001365
9	1	.000004018	.000001039	.000002024
10	1	.000002650	-.000005548	-.000002360
11	1	.000003892	.000006282	-.000003396
12	1	-.000000834	-.000001909	.000001090
13	1	.000007230	.000011464	-.000001647
14	1	-.000000173	-.000001238	.000008786
15	1	.000002135	.000004258	-.000003795
16	1	-.000014305	-.000031029	-.000010299
17	1	-.000002426	-.000005942	.000002545
18	1	.000000048	-.000000342	-.000000370
19	1	-.000013856	.000024184	-.000014264
20	1	-.000004586	.000016068	.000008252
21	1	-.000006228	-.000016957	.000010434

Cartesian Forces: Max .000031029 RMS .000008291
1\1\GINC-ESHEL\Freq\RMP2-FC\6-31G(d)\C7H13N1\BELOSTOT\19-Oct-2002\0\#
MP2/6-31G* OPT=(CARTESIAN, NEWTON, TS, CALCALL)\1-Azabicyclo4.2.0octan
e, RINI transition state\0,1\C,-1.6935070308,0.7412980808,-0.71993091
58\C,-1.7026121154,0.6641568278,0.8133926622\C,-0.2825413524,0.7275211
796,1.3948630811\C,-0.8728105008,-0.4026855949,-1.3308428699\C,0.50954
72781,-0.4380977136,0.8216478656\N,0.3586735612,-0.5117307819,-0.61246
8271\C,2.0398582635,-0.3324807573,0.585875239\C,1.7688193629,-0.579203
3746,-0.9263907801\H,-2.7205155946,0.7185259517,-1.106362391\H,-2.3157
337996,1.4765015248,1.2208052161\H,-2.1788322272,-0.2760335993,1.12726
03655\H,0.1937233017,1.6687160615,1.0897764929\H,-1.4641381251,-1.3377
699983,-1.2924112235\H,-0.6555400559,-0.2059279791,-2.3879130967\H,0.2
192838536,-1.3674622001,1.3526665267\H,2.4362917923,0.6639122196,0.798
5915085\H,-1.2473983167,1.6962314292,-1.024178921\H,-0.3041581813,0.70
04935201,2.4920215087\H,2.6545894847,-1.0813449147,1.0908724447\H,2.12
93630465,-1.5548650707,-1.2942491502\H,2.1418264632,0.198086642,-1.611
2870756\Version=IBM-RS6000-G98RevA.7\HF=-327.0464948\MP2=-328.1187854
\RMSD=3.298e-09\RMSF=8.291e-06\Dipole=0.0462451,0.123647,0.0047729\

Conformation 7 (RI transition state)

Item Value Threshold Converged?
 Maximum Force .000036 .000450 YES
 RMS Force .000010 .000300 YES
 Maximum Displacement .001620 .001800 YES
 RMS Displacement .000477 .001200 YES
 Predicted change in Energy=-1.329303D-08

Optimization completed.

-- Stationary point found.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.876910	-.552879	-.066342
2	6	0	1.525297	.754980	.636095
3	6	0	.559578	1.529783	-.254943
4	6	0	.661212	-1.473431	-.083914
5	6	0	-.660306	.688622	-.639285
6	7	0	-.558542	-.804568	-.537597
7	6	0	-1.852398	.673949	.341370
8	6	0	-1.729103	-.860015	.364494
9	1	0	2.205420	-.334458	-1.090478
10	1	0	1.070297	.537755	1.612334
11	1	0	2.422311	1.354385	.828906
12	1	0	.217107	2.457376	.222014
13	1	0	.861573	-2.354903	-.709224
14	1	0	.510671	-1.846340	.943341
15	1	0	-.975086	.962323	-1.655690
16	1	0	-1.626576	1.145934	1.302898
17	1	0	2.705256	-1.071038	.430431
18	1	0	1.104219	1.825772	-1.160304
19	1	0	-2.789676	1.087121	-.040757
20	1	0	-2.577518	-1.411769	-.059043
21	1	0	-1.505344	-1.286237	1.353906

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.860973	-.604566	-.064392
2	6	0	1.544374	.710440	.641347
3	6	0	.602333	1.514417	-.249192
4	6	0	.620234	-1.490960	-.087126
5	6	0	-.639648	.708598	-.638459
6	7	0	-.579569	-.787140	-.541129
7	6	0	-1.833666	.724085	.339835
8	6	0	-1.753038	-.812773	.358519
9	1	0	2.197487	-.392282	-1.087219
10	1	0	1.081548	.503006	1.616036
11	1	0	2.457286	1.284134	.837723
12	1	0	.284774	2.449726	.229928
13	1	0	.797317	-2.375778	-.714733
14	1	0	.457326	-1.862621	.938693
15	1	0	-.944655	.993974	-1.654633
16	1	0	-1.596775	1.186738	1.303234
17	1	0	2.673614	-1.147005	.432401
18	1	0	1.156806	1.797884	-1.152589
19	1	0	-2.758342	1.164257	-.042845
20	1	0	-2.615582	-1.339493	-.068341
21	1	0	-1.543194	-1.248003	1.347058

Rotational constants (GHZ): 3.2793010 2.1099147 1.5284776

Isotopes: C-12,C-12,C-12,C-12,C-12,N-14,C-12,C-12,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1

Rotating electric field derivatives to standard orientation.

Rotating nuclear coordinate derivatives to standard orientation.

S100

Full mass-weighted force constant matrix:

Low frequencies --- -98.0541 -2.2432 -1.7923 -.9197 -.0004 .0003

Low frequencies --- .0009 101.8263 292.2506

***** 1 imaginary frequencies (negative Signs) *****

Harmonic frequencies (cm⁻¹), IR intensities (KM/Mole),Raman scattering activities (A⁴/AMU), Raman depolarization ratios,

reduced masses (AMU), force constants (mDyne/A) and normal coordinates:

1 ?A				2 ?A				3 ?A			
Frequencies --	-98.0540				101.8263				292.2506		
Red. masses --	2.0296				2.1389				2.0127		
Frc consts --	.0115				.0131				.1013		
IR Inten --	.4197				.2635				.1543		
Raman Activ --	.0000				.0000				.0000		
Depolar --	.0000				.0000				.0000		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z		
1 6	-.01	.00	.01	.00	.01	.13	.05	-.07	.12		
2 6	.05	.05	-.05	-.12	.02	.05	.14	.05	-.06		
3 6	.01	.01	-.05	.01	-.03	-.14	.03	-.02	-.02		
4 6	-.03	.03	.13	.01	-.01	-.12	-.03	.03	-.06		
5 6	-.01	.01	.05	-.03	.00	-.03	-.05	.05	.07		
6 7	.01	.00	-.04	-.02	.00	-.05	-.03	.05	-.04		
7 6	.06	-.04	.13	.10	.01	.12	-.13	-.04	.00		
8 6	-.09	-.05	-.17	.04	.01	.03	.00	-.04	.00		
9 1	-.04	-.08	-.01	.20	.01	.20	.30	-.21	.18		
10 1	.10	.11	-.02	-.28	.06	-.01	.30	.22	.05		
11 1	.07	.05	-.14	-.15	.03	.18	.19	.06	-.31		
12 1	.04	.03	-.08	.06	.08	-.32	.13	.03	-.04		
13 1	-.04	-.07	.27	.09	.11	-.26	-.01	.09	-.14		
14 1	-.05	.20	.19	-.06	-.21	-.20	-.11	-.08	-.11		
15 1	-.11	.03	.08	-.14	.02	.01	-.06	.11	.09		
16 1	.21	-.27	.20	.26	-.05	.11	-.31	.00	.02		
17 1	.00	.01	.02	-.10	.01	.29	-.12	-.13	.34		
18 1	-.03	-.04	-.09	.09	-.23	-.16	-.07	-.10	-.10		
19 1	.08	.15	.30	.07	.08	.27	-.13	-.16	-.13		
20 1	-.10	.14	-.38	-.01	.07	.05	.03	-.13	.06		
21 1	-.25	-.29	-.24	.08	-.06	-.01	.09	.01	.00		

4 ?A				5 ?A				6 ?A			
Frequencies --	350.6261				384.5609				430.5873		
Red. masses --	2.7622				1.8296				2.8993		
Frc consts --	.2001				.1594				.3167		
IR Inten --	5.2606				.1652				.6338		
Raman Activ --	.0000				.0000				.0000		
Depolar --	.0000				.0000				.0000		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z		
1 6	.07	.01	-.03	.03	-.01	-.06	-.01	.16	-.03		
2 6	-.01	-.01	-.02	-.07	-.08	.03	.12	.07	.16		
3 6	.03	.00	-.06	.08	-.04	-.08	.10	-.15	.00		
4 6	.09	-.06	-.08	.00	.06	.06	.00	.09	-.05		
5 6	.00	-.01	.05	-.03	.08	.06	.02	-.10	.04		
6 7	.07	.07	.27	.04	.08	-.02	-.13	-.10	-.06		
7 6	-.08	.02	-.02	-.10	-.03	.02	-.01	.01	-.02		
8 6	-.14	.00	-.05	.06	-.03	-.01	-.12	.00	.02		
9 1	.07	.04	-.02	-.06	.05	-.08	-.18	.35	-.05		
10 1	-.09	-.04	-.07	-.27	-.21	-.09	.20	.08	.19		
11 1	-.04	.00	.06	-.12	-.09	.29	.13	.11	.03		
12 1	.11	.06	-.13	.27	.12	-.27	.10	.02	-.32		
13 1	.06	.12	-.35	-.11	-.06	.21	.13	.13	-.07		
14 1	.20	-.35	-.16	.03	.26	.14	.06	.03	-.06		
15 1	.01	-.13	.01	-.08	.11	.08	.07	.00	.05		
16 1	-.08	-.05	.02	-.28	.00	.05	-.08	.05	-.02		
17 1	.09	.04	-.03	.07	-.02	-.14	.07	.02	-.30		
18 1	.01	-.12	-.11	.12	-.34	-.15	.16	-.44	-.05		
19 1	-.03	.11	-.04	-.10	-.16	-.10	.04	.04	-.12		
20 1	-.05	.10	-.37	.10	-.13	.03	-.16	.05	.06		
21 1	-.48	-.11	-.03	.15	.00	-.01	-.11	.01	.02		

7 ?A				8 ?A				9 ?A			
Frequencies --	477.9037				623.8417				645.9920		
Red. masses --	2.9964				2.3509				2.8625		

S101

Frc consts --	.4032	.5391	.7038
IR Inten --	.4397	4.4061	.7530
Raman Activ --	.0000	.0000	.0000
Depolar --	.0000	.0000	.0000
Atom AN	X Y Z	X Y Z	X Y Z
1 6	.24 -.01 -.01	.08 .01 -.03	.00 .02 -.02
2 6	.01 -.11 -.01	-.03 .03 -.08	.05 .00 .00
3 6	-.12 -.16 .04	.07 .13 -.02	.12 .08 -.02
4 6	.10 .14 .01	.05 -.04 -.01	-.12 .17 -.05
5 6	-.12 -.04 -.08	.08 -.02 .14	.06 -.02 -.11
6 7	-.04 .01 -.03	-.08 -.14 -.09	-.10 .06 .11
7 6	-.02 .08 .02	-.01 .02 .03	.05 -.14 -.06
8 6	-.06 .07 .01	-.11 .02 .03	-.07 -.14 .07
9 1	.47 -.07 .05	.29 -.12 .02	.28 -.06 .05
10 1	.02 -.30 -.05	-.36 -.12 -.26	-.17 -.11 -.12
11 1	-.15 .11 .09	-.07 -.05 .34	.04 -.08 .28
12 1	-.13 -.23 .18	.02 .04 .12	.02 -.02 .11
13 1	.00 .02 .15	.08 -.09 .06	-.17 .09 .05
14 1	.14 .31 .08	.10 .04 .03	-.01 .26 .01
15 1	-.10 .00 -.08	.02 .00 .17	.15 -.06 -.16
16 1	.18 .07 -.03	-.31 .09 .07	.27 -.23 -.07
17 1	.07 -.08 .20	-.04 .07 .22	-.24 -.16 .18
18 1	-.12 .00 .09	-.05 .26 -.06	.13 .25 .05
19 1	-.06 .14 .17	.10 -.01 -.27	.01 -.01 .17
20 1	-.08 .14 -.02	-.17 .08 .09	-.02 -.23 .07
21 1	-.10 .03 .00	-.09 .03 .03	-.04 -.09 .09
	10	11	12
	?A	?A	?A
Frequencies --	757.2807	816.7661	849.9033
Red. masses --	2.4852	1.2629	1.4054
Frc consts --	.8397	.4964	.5981
IR Inten --	1.7113	.9020	.7200
Raman Activ --	.0000	.0000	.0000
Depolar --	.0000	.0000	.0000
Atom AN	X Y Z	X Y Z	X Y Z
1 6	.08 -.03 .04	.00 .01 -.04	.00 .01 .05
2 6	.07 -.01 .05	-.04 .01 -.01	.04 .01 -.04
3 6	.08 .12 -.02	-.04 .00 .05	.03 -.08 -.06
4 6	.08 -.11 .06	.01 -.03 -.02	-.03 .05 .04
5 6	-.11 .13 -.14	.02 .01 .08	.02 -.07 .04
6 7	-.05 -.06 -.05	.01 .00 .00	.01 .03 .00
7 6	-.11 -.02 -.01	.01 .01 -.07	-.04 .04 .01
8 6	-.07 .00 .03	-.04 -.01 -.03	.02 .01 -.06
9 1	-.24 .06 -.05	.17 -.03 .01	-.26 .01 -.03
10 1	-.01 .02 .03	.09 -.03 .04	-.25 .02 -.17
11 1	.07 -.03 .13	-.02 .02 -.11	-.04 .05 .23
12 1	.19 .12 .05	.08 .15 -.16	-.14 -.29 .24
13 1	.13 -.03 -.05	-.05 -.10 .06	.08 .20 -.15
14 1	-.01 -.22 .00	.06 .08 .03	-.14 -.20 -.07
15 1	-.06 .07 -.17	.08 .01 .06	-.04 -.05 .07
16 1	.25 -.23 .00	.21 -.34 .05	-.02 -.19 .11
17 1	.30 .04 -.23	-.06 .06 .13	.10 -.04 -.17
18 1	.13 .12 .01	-.02 -.26 -.03	-.14 .30 -.04
19 1	-.24 .11 .44	.13 .42 .11	.05 .25 .04
20 1	-.05 -.13 .14	.06 -.37 .21	.09 -.25 .12
21 1	-.02 .16 .09	.13 .39 .12	.19 .24 .01
	13	14	15
	?A	?A	?A
Frequencies --	899.6907	908.3970	959.0763
Red. masses --	2.5611	2.3753	1.3564
Frc consts --	1.2214	1.1548	.7351
IR Inten --	3.1347	.4820	.1300
Raman Activ --	.0000	.0000	.0000
Depolar --	.0000	.0000	.0000
Atom AN	X Y Z	X Y Z	X Y Z
1 6	.11 -.10 -.07	.14 -.07 .04	-.03 .02 -.03
2 6	.10 .14 .15	-.02 .03 -.01	.07 .02 -.04
3 6	-.08 .09 -.03	-.09 -.01 -.01	-.04 .02 .07
4 6	-.11 -.09 -.06	-.03 -.01 .04	-.02 .04 .07
5 6	-.01 -.10 .00	.01 .09 .04	-.04 .00 .01
6 7	.01 .02 .02	-.05 .09 -.03	.00 -.03 -.01

S102

7	6	-.04	.04	.03	.18	-.07	-.08	.01	-.01	-.04
8	6	.06	.03	-.05	-.09	-.08	.06	.04	.02	-.01
9	1	.13	-.05	-.06	-.28	.00	-.09	-.04	-.38	-.11
10	1	-.07	-.02	.04	-.03	.03	-.01	-.04	-.39	-.18
11	1	.02	.19	.41	-.17	.25	.00	-.02	.04	.31
12	1	-.35	.13	-.30	.00	.04	-.05	.09	.19	-.18
13	1	-.36	-.26	.10	-.13	.08	-.11	.19	.26	-.18
14	1	-.09	.12	.03	-.19	-.18	-.05	-.11	-.31	-.07
15	1	-.04	-.16	-.01	-.05	.23	.10	.08	-.01	-.02
16	1	.00	.03	.02	-.03	.07	-.10	.15	.05	-.10
17	1	.04	-.27	-.14	.39	-.01	-.29	-.12	.01	.11
18	1	-.09	.00	-.07	-.13	-.09	-.06	-.09	-.29	-.06
19	1	-.05	.03	.04	.30	-.06	-.35	-.06	-.06	.08
20	1	.07	.01	-.03	-.13	-.03	.08	.02	.10	-.06
21	1	.11	.00	-.07	-.06	-.08	.06	-.01	-.05	-.03

16

17

18

?A

?A

?A

Frequencies --	984.7963	1016.0942	1047.9103
Red. masses --	2.3279	2.3790	1.9608
Frc consts --	1.3302	1.4472	1.2686
IR Inten --	.9704	2.2977	2.4405
Raman Activ --	.0000	.0000	.0000
Depolar --	.0000	.0000	.0000

Atom AN		X			Y			Z		
1	6	.06	.09	-.04	.01	.04	.00	.08	-.04	.00
2	6	-.04	.11	-.07	.00	.02	-.02	-.10	-.05	-.02
3	6	.07	-.15	.07	.04	-.02	.03	-.01	.09	.01
4	6	-.08	-.14	.01	-.01	-.06	.01	-.01	.08	.06
5	6	.09	.03	-.04	-.05	.01	-.01	.13	-.10	-.06
6	7	-.05	.05	.01	-.04	.00	.00	-.03	.03	-.03
7	6	-.05	-.06	.03	-.02	.23	.00	-.06	.03	.09
8	6	.02	.06	-.01	.03	-.24	.00	-.03	-.01	-.01
9	1	.12	-.05	-.05	.04	-.01	.00	-.09	-.15	-.08
10	1	-.09	-.01	-.12	-.02	-.02	-.04	.29	-.16	.14
11	1	-.22	.35	.02	-.02	.04	.03	-.07	.00	-.30
12	1	.07	-.18	.12	.12	-.01	.07	-.16	.17	-.25
13	1	-.23	-.17	.02	-.05	-.07	.02	-.04	.24	-.17
14	1	-.13	-.09	.03	-.01	-.04	.02	-.11	-.20	-.06
15	1	.30	.15	-.07	.05	.00	-.04	.17	-.20	-.10
16	1	.01	-.11	.03	.14	.47	-.14	-.20	-.02	.16
17	1	.12	.38	.17	.05	.17	.08	.19	.13	-.01
18	1	.11	-.07	.12	.05	-.02	.04	.33	-.07	.16
19	1	-.21	-.22	.22	.06	.36	-.07	-.05	.01	.02
20	1	-.02	.11	.01	.10	-.30	-.08	-.03	-.10	.09
21	1	.03	.00	-.04	.18	-.49	-.13	.18	-.06	-.08

19

20

21

?A

?A

?A

Frequencies --	1055.9438			1085.7546			1101.4097		
Red. masses --	1.6838			2.8392			1.6215		
Frc consts --	1.1062			1.9720			1.1589		
IR Inten --	3.2042			21.2505			2.7265		
Raman Activ --	.0000			.0000			.0000		
Depolar --	.0000			.0000			.0000		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	.01	-.08	.05	-.11	.00	-.02	-.04	-.11	-.07
2 6	-.05	.02	-.05	.06	.04	.02	-.05	.10	.03
3 6	.00	.02	.05	-.02	-.06	-.02	.01	-.05	.01
4 6	.02	.06	-.05	.12	-.07	.00	.05	.05	.01
5 6	.05	-.08	.08	.05	-.04	-.05	.04	.08	-.03
6 7	.04	.02	-.07	.13	.18	-.11	.02	-.05	.00
7 6	-.08	.01	-.05	-.03	-.01	.04	-.02	.03	.02
8 6	.00	.00	.09	-.17	-.04	.12	-.01	-.03	.02
9 1	-.19	.09	.01	-.04	-.28	-.06	-.02	-.31	-.10
10 1	-.20	.28	-.07	.00	-.20	-.06	-.06	.17	.04
11 1	-.02	-.02	-.03	.18	-.22	.22	-.26	.45	-.05
12 1	.17	.08	.03	-.49	-.10	-.24	.00	-.08	.06
13 1	-.05	-.02	.05	.13	-.13	.09	.23	.09	-.02
14 1	-.06	.17	-.03	-.05	.06	.01	.15	-.02	.00
15 1	.39	-.11	-.02	.05	.26	.01	.06	.12	-.03
16 1	.34	.07	-.18	-.02	.08	.00	-.11	-.04	.08
17 1	.13	-.11	-.19	-.11	.20	.19	-.27	-.49	-.11

S103

18	1	-.20	-.13	-.13	.00	.05	.03	.16	.03	.13
19	1	-.22	.02	.30	.00	.04	.00	.00	.06	.00
20	1	.04	.13	-.15	-.14	-.08	.12	.05	-.08	-.04
21	1	-.15	-.18	.04	-.08	-.04	.10	-.09	.01	.05
	22				23			24		
	?A				?A			?A		
Frequencies --		1161.6094			1163.8942			1187.6259		
Red. masses --		1.7129			1.3823			1.9137		
Frc consts --		1.3618			1.1033			1.5903		
IR Inten --		13.2232			3.1657			2.5221		
Raman Activ --		.0000			.0000			.0000		
Depolar --		.0000			.0000			.0000		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z	
1	6	.00	-.01	-.01	-.02	-.03	.00	-.02	.00	.12
2	6	.01	-.04	.02	.00	.03	-.02	.06	-.01	-.09
3	6	-.07	-.03	-.06	.01	.01	.06	-.08	.00	.07
4	6	.05	-.01	.04	.05	.00	.00	.01	.00	-.11
5	6	.11	.11	.04	-.04	-.05	-.03	.06	.04	-.11
6	7	-.11	-.01	.04	.01	.04	.04	-.03	-.04	.06
7	6	-.01	.02	-.03	.03	-.01	.03	.02	.04	.09
8	6	.04	-.02	-.04	-.07	.01	-.10	.00	-.01	-.02
9	1	.09	.13	.06	-.01	.02	.01	-.24	.09	.06
10	1	-.03	.06	.02	-.15	.18	-.05	-.10	-.16	-.20
11	1	.13	-.22	.00	.01	-.01	.04	-.01	.01	.16
12	1	-.43	-.07	-.21	.25	.07	.08	.08	.14	-.11
13	1	.07	.07	-.05	.03	-.01	.00	.25	-.21	.24
14	1	.27	-.07	.06	.16	.02	.03	-.15	.32	-.01
15	1	.39	.24	-.01	.04	-.10	-.07	.18	.06	-.14
16	1	.06	-.05	-.01	.03	.17	-.06	-.32	-.10	.23
17	1	-.04	-.08	-.01	-.05	-.12	-.05	.11	-.04	-.15
18	1	-.28	.05	-.16	-.08	-.11	-.03	-.13	-.23	-.04
19	1	-.18	-.12	.20	-.02	-.18	-.02	.07	-.01	-.10
20	1	-.07	.06	.07	-.40	.08	.45	.13	-.18	-.07
21	1	.18	-.16	-.13	.51	-.02	-.23	-.07	.09	.05
	25				26			27		
	?A				?A			?A		
Frequencies --		1211.1128			1236.3093			1256.4110		
Red. masses --		2.0266			1.2968			1.2367		
Frc consts --		1.7514			1.1679			1.1502		
IR Inten --		16.8154			3.1596			.4556		
Raman Activ --		.0000			.0000			.0000		
Depolar --		.0000			.0000			.0000		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z	
1	6	.01	.10	.01	.00	.00	-.05	.01	-.01	.02
2	6	.04	-.08	.02	.01	.00	.01	-.02	.00	.00
3	6	-.07	.01	-.09	-.03	-.01	.03	.03	.00	-.02
4	6	-.11	-.04	.00	-.02	.00	.07	.00	.01	-.04
5	6	.08	.08	.03	.01	.00	-.06	-.01	.00	.06
6	7	.13	-.02	-.03	.03	.00	-.05	-.01	-.02	.03
7	6	-.03	.01	.02	.04	.02	.07	.05	.03	.01
8	6	-.08	-.03	.03	-.04	-.01	-.01	-.03	-.03	-.08
9	1	.13	.23	.08	.20	.20	.06	-.10	-.13	-.05
10	1	.19	-.30	.05	-.18	.27	-.02	.10	-.11	.03
11	1	-.22	.36	-.04	.11	-.17	.03	-.03	.04	-.04
12	1	.20	-.02	.15	.13	.04	.04	-.15	-.04	-.05
13	1	.14	-.03	.04	-.28	.14	-.19	.13	-.05	.08
14	1	-.10	-.07	.00	.20	-.20	.03	-.15	.11	-.03
15	1	.19	-.35	-.11	.15	-.11	-.13	-.02	.07	.08
16	1	.04	.11	-.04	-.12	.17	.04	.19	.38	-.19
17	1	-.18	-.26	-.07	-.06	-.03	.03	.06	.05	.00
18	1	-.11	.08	-.10	-.21	-.09	-.11	.10	.08	.05
19	1	-.10	-.05	.11	-.02	-.19	-.01	-.27	-.47	.21
20	1	-.19	.03	.19	.22	-.31	-.15	.06	-.26	.01
21	1	.08	-.05	-.01	-.21	.27	.15	-.12	.37	.12
	28				29			30		
	?A				?A			?A		
Frequencies --		1294.0958			1299.1686			1306.3840		
Red. masses --		1.5226			2.0567			1.3296		
Frc consts --		1.5024			2.0453			1.3369		
IR Inten --		8.2401			26.6421			8.3038		
Raman Activ --		.0000			.0000			.0000		

S104

Depolar	--	.0000			.0000			.0000		
Atom AN		X	Y	Z	X	Y	Z	X	Y	Z
1	6	.00	-.01	.00	.05	-.01	.00	.02	.04	.00
2	6	.00	.01	.01	-.02	.02	-.06	-.01	-.03	-.05
3	6	.00	.00	.01	.03	-.03	.07	.01	.04	.03
4	6	-.01	.02	-.01	-.12	.07	-.01	-.02	-.05	.05
5	6	-.01	-.01	.00	-.01	.07	-.03	.03	-.09	-.02
6	7	.04	-.02	-.01	.16	-.13	.04	-.02	.04	.00
7	6	.09	.14	-.11	-.04	.00	.01	.00	.01	-.02
8	6	-.03	-.03	.04	-.02	-.04	-.01	-.02	.04	.02
9	1	-.03	-.05	-.02	.06	.20	.04	.20	.31	.11
10	1	-.02	.03	.00	-.18	.19	-.10	-.04	.04	-.06
11	1	.02	-.02	.02	.14	-.26	-.01	-.07	.07	-.06
12	1	.03	-.01	.04	-.41	.00	-.28	-.01	.08	-.07
13	1	-.14	.01	-.04	-.11	.09	-.05	.27	-.01	.05
14	1	.01	.00	-.01	-.14	-.06	-.06	-.09	-.11	.02
15	1	-.20	-.06	.05	-.10	.36	.07	-.28	.48	.22
16	1	-.36	-.49	.30	.05	.11	-.06	.06	.00	-.03
17	1	.05	.11	.04	.09	.02	-.04	-.17	-.39	-.15
18	1	-.02	-.04	-.01	.15	-.05	.14	.06	-.06	.03
19	1	-.34	-.38	.32	.02	.14	.00	-.08	-.08	.07
20	1	-.05	.00	.03	-.28	.18	.23	.18	-.17	-.12
21	1	.07	-.18	-.04	.01	.06	.03	.09	-.11	-.07

31

32

33

?A

?A

?A

Frequencies -- 1318.6048 1347.8759 1368.6688

Red. masses -- 1.2097 1.4596 1.3084

Frc consts -- 1.2392 1.5623 1.4441

IR Inten -- .7196 8.5170 7.8732

Raman Activ -- .0000 .0000 .0000

Depolar -- .0000 .0000 .0000

Atom AN		X	Y	Z	X	Y	Z	X	Y	Z
1	6	-.05	-.02	.09	.01	.02	.00	.01	-.02	-.01
2	6	.04	.01	-.07	.00	.00	-.05	.01	.00	-.03
3	6	-.01	.00	.00	.02	.00	.03	.02	-.03	.03
4	6	.02	.00	-.01	.03	-.04	.04	-.03	-.01	-.01
5	6	.00	.00	.02	-.05	-.01	.03	-.05	.07	.05
6	7	.00	.00	-.02	-.04	.08	-.03	.00	.01	-.01
7	6	-.01	-.01	-.01	.02	.03	-.01	.03	-.03	-.01
8	6	.00	.00	.00	.08	-.10	-.02	-.06	.08	.03
9	1	-.11	.20	.11	.13	.21	.08	.06	.10	.03
10	1	.07	-.30	-.12	-.07	.03	-.08	-.14	.14	-.07
11	1	-.12	.21	.07	.02	-.04	-.02	.04	-.06	.01
12	1	-.11	.02	-.10	-.18	.01	-.13	-.28	-.03	-.17
13	1	-.46	.02	-.14	.17	-.01	.03	.32	-.01	.08
14	1	.58	.02	.10	-.13	-.03	.01	.04	.00	.01
15	1	-.10	.00	.05	.13	-.33	-.11	.02	-.53	-.13
16	1	.07	.05	-.05	-.11	-.13	.10	.03	.01	-.03
17	1	.00	-.07	-.06	-.11	-.26	-.12	.05	.04	-.01
18	1	.28	.00	.17	.23	-.02	.15	.25	.00	.18
19	1	-.02	-.02	.02	-.02	-.02	.01	.04	-.04	-.03
20	1	.02	-.01	-.03	-.27	.34	.13	.25	-.26	-.15
21	1	.01	.02	.00	-.33	.26	.23	.23	-.23	-.17

34

35

36

?A

?A

?A

Frequencies -- 1389.5008 1413.1766 1425.7176

Red. masses -- 1.3707 1.5687 1.5681

Frc consts -- 1.5592 1.8458 1.8780

IR Inten -- .7465 3.1518 .3778

Raman Activ -- .0000 .0000 .0000

Depolar -- .0000 .0000 .0000

Atom AN		X	Y	Z	X	Y	Z	X	Y	Z
1	6	.05	.06	.03	-.01	-.03	.01	.07	.16	.05
2	6	-.07	.11	-.02	-.05	.01	-.01	-.01	-.09	.00
3	6	-.03	-.03	-.04	.16	.02	.04	.05	.02	.04
4	6	.02	-.01	.00	.00	.01	.00	-.03	-.05	-.03
5	6	-.04	.01	.02	-.13	-.02	-.01	-.01	.00	-.01
6	7	.01	-.02	.00	.03	-.01	.00	.01	.01	-.01
7	6	.02	.00	.00	.03	.01	.01	.00	.00	.00
8	6	-.02	.03	.01	-.01	.02	.01	.00	.00	.01
9	1	-.04	-.10	-.03	.01	.19	.07	-.29	-.59	-.22

S105

10	1	.16	-.31	.00	.25	-.30	.07	-.11	.29	.03
11	1	.30	-.50	.01	-.17	.21	-.08	-.04	-.01	-.12
12	1	.16	-.07	.15	-.28	-.02	-.16	-.24	.00	-.12
13	1	-.21	-.05	.00	-.03	-.01	.01	-.14	-.06	-.04
14	1	-.14	-.04	-.03	-.03	-.04	-.01	.30	.07	.07
15	1	.26	.06	-.05	.42	.12	-.14	-.05	-.08	-.02
16	1	-.02	-.04	.03	-.10	-.10	.09	-.03	.01	.00
17	1	-.12	-.41	-.18	-.02	-.05	-.01	-.17	-.30	-.05
18	1	.19	.03	.12	-.43	.11	-.30	-.14	-.06	-.09
19	1	.02	-.03	-.03	.08	.00	-.10	.01	.02	.00
20	1	.08	-.09	-.04	.05	-.04	-.04	.01	.00	-.02
21	1	.08	-.08	-.06	.06	-.03	-.03	-.01	.01	.01

37

38

39

?A

?A

?A

Frequencies -- 1433.3732 1441.5261 1543.9833

Red. masses -- 1.4338 1.3706 1.1001

Frc consts -- 1.7356 1.6781 1.5451

IR Inten -- 2.1751 15.4139 .6023

Raman Activ -- .0000 .0000 .0000

Depolar -- .0000 .0000 .0000

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	.04	-.04	.01	-.02	.01	.00	.03	-.01	-.01
2	6	-.07	.09	.00	-.02	.02	-.01	.00	.00	-.01
3	6	.04	-.03	.03	.05	-.02	.06	-.01	-.04	.01
4	6	-.10	-.01	-.01	.11	.02	.01	.00	.00	.00
5	6	.06	.02	-.03	.08	.06	-.02	.01	.01	.00
6	7	-.01	.03	-.02	-.03	-.02	.01	.00	.00	.00
7	6	-.02	.00	.00	-.02	-.02	-.01	-.04	.05	.03
8	6	.01	-.02	.00	.00	.01	-.01	.01	.01	.00
9	1	-.03	.03	.00	.04	.09	.04	-.26	.14	-.07
10	1	.21	-.28	.05	.01	-.11	-.03	.03	.04	.02
11	1	.14	-.25	.02	-.01	.02	-.05	.00	-.03	.05
12	1	.03	-.05	.07	-.14	-.02	-.09	.15	.16	-.23
13	1	.42	.05	.04	-.40	-.06	-.01	.00	.00	-.01
14	1	.44	.02	.10	-.46	-.05	-.11	.01	.00	.00
15	1	-.40	-.19	.05	-.47	-.37	.03	-.04	-.03	.01
16	1	.02	.04	-.03	.03	.10	-.07	.43	-.30	.06
17	1	.09	-.02	-.05	-.11	-.16	-.05	-.16	-.04	.25
18	1	-.30	-.05	-.18	-.26	-.05	-.14	-.07	.30	.07
19	1	-.03	.03	.04	-.03	.04	.06	.00	-.30	-.42
20	1	-.04	.07	.01	.01	-.07	.06	-.02	-.09	.15
21	1	-.07	.07	.05	-.02	-.08	-.03	-.15	-.10	-.01

40

41

42

?A

?A

?A

Frequencies -- 1546.6181 1554.7564 1562.2169

Red. masses -- 1.0905 1.0874 1.0947

Frc consts -- 1.5369 1.5487 1.5740

IR Inten -- 3.7170 7.3047 4.8994

Raman Activ -- .0000 .0000 .0000

Depolar -- .0000 .0000 .0000

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-.04	.01	.02	.03	-.01	-.02	-.04	.02	.02
2	6	-.01	-.01	-.02	-.02	-.02	-.07	-.02	-.02	-.04
3	6	.01	.04	-.01	.00	.01	-.01	-.01	-.05	.02
4	6	.00	.00	.00	.01	.00	.00	.00	-.01	.00
5	6	.00	.01	.00	.00	.01	.00	.00	.00	.00
6	7	.01	.00	.00	.00	.00	.00	.00	.00	.00
7	6	-.03	.03	.02	.01	-.01	-.01	.01	-.01	-.01
8	6	.00	.01	.00	.00	.00	.00	.00	.00	.00
9	1	.32	-.18	.08	-.27	.20	-.07	.31	-.21	.08
10	1	.14	.10	.08	.43	.29	.23	.27	.18	.15
11	1	-.05	.00	.18	-.11	-.05	.56	-.08	-.03	.32
12	1	-.20	-.19	.27	-.09	-.10	.13	.20	.21	-.34
13	1	-.02	.04	-.06	.00	.00	-.02	-.01	.08	-.11
14	1	-.01	.06	.02	-.05	.01	.00	-.03	.13	.04
15	1	-.01	-.01	-.01	.00	-.01	.00	-.02	-.01	.01
16	1	.32	-.20	.04	-.09	.07	-.02	-.08	.05	-.01
17	1	.19	.04	-.31	-.19	-.05	.28	.18	.02	-.32
18	1	.06	-.38	-.10	.06	-.18	-.03	-.10	.44	.10
19	1	.01	-.21	-.32	.00	.06	.09	-.01	.05	.08
20	1	-.01	-.08	.12	.01	.02	-.05	.00	.01	-.01

S106

```

21 1  -.11  -.09  -.01  .05  .03  .00  .02  .01  .00
      43      44      45
      ?A      ?A      ?A
Frequencies -- 1576.4172      1595.4668      3025.9500
Red. masses -- 1.0992      1.0971      1.0668
Frc consts -- 1.6094      1.6454      5.7549
IR Inten -- 2.3011      4.4152      48.3746
Raman Activ -- .0000      .0000      .0000
Depolar -- .0000      .0000      .0000
Atom AN  X   Y   Z   X   Y   Z   X   Y   Z
 1 6  -.01  .01  .00  -.01  .00  .01  .00  .00  .00
 2 6  .00  -.01  -.01  .00  -.01  -.01  .00  .00  .00
 3 6  .00  -.01  .00  .00  .00  .00  .00  .00  .00
 4 6  .01  .05  -.01  -.01  .06  -.02  .01  .05  -.06
 5 6  .01  .01  .00  -.01  -.01  .00  .00  .00  .00
 6 7  -.01  .00  .00  .00  .01  -.01  .00  .00  .00
 7 6  -.02  .02  .01  .01  -.01  -.01  .00  .00  .00
 8 6  -.03  -.05  .03  .03  .04  -.03  .00  .00  .00
 9 1  .06  -.06  .01  .03  -.05  .01  .01  .01  -.04
10 1  .04  .05  .03  .06  .06  .03  .01  .01  -.01
11 1  -.02  .00  .06  -.02  .00  .08  .00  .00  .00
12 1  .01  .02  -.03  .03  .02  -.02  .00  .00  .00
13 1  -.06  -.26  .37  -.02  -.28  .42  .05  -.24  -.21
14 1  .07  -.43  -.15  .17  -.48  -.16  -.15  -.30  .88
15 1  -.03  -.02  .00  .03  .02  .01  .01  .00  .02
16 1  .15  -.10  .02  -.11  .07  -.01  .00  .00  .00
17 1  .03  .01  -.07  .04  .02  -.05  -.03  .02  -.02
18 1  -.02  .03  .00  .01  .04  .02  .00  .00  .00
19 1  -.01  -.10  -.14  .00  .07  .11  .00  .00  .00
20 1  .02  .27  -.41  -.02  -.23  .37  .03  .02  .02
21 1  .39  .31  .07  -.38  -.24  -.04  -.02  .02  -.05
      46      47      48
      ?A      ?A      ?A
Frequencies -- 3058.2730      3072.2175      3084.4438
Red. masses -- 1.0627      1.0826      1.0895
Frc consts -- 5.8563      6.0205      6.1068
IR Inten -- 74.2961      23.0840      37.7335
Raman Activ -- .0000      .0000      .0000
Depolar -- .0000      .0000      .0000
Atom AN  X   Y   Z   X   Y   Z   X   Y   Z
 1 6  .00  .00  .00  .00  .00  .00  -.02  .00  .02
 2 6  .00  .00  .00  .00  .00  .00  .00  .00  .00
 3 6  .00  .00  .00  -.01  -.02  .02  .00  -.01  .00
 4 6  .00  .00  .01  .00  .00  .01  .01  -.05  -.06
 5 6  .00  .00  .01  -.02  .02  -.07  .00  .00  .00
 6 7  .00  .00  .00  .00  .00  .00  .00  .00  .00
 7 6  .00  .00  -.01  .00  .00  .00  .00  .00  .00
 8 6  -.01  -.05  .05  .00  -.01  .01  .00  .00  .00
 9 1  .00  .00  .01  .00  .00  .01  .11  .07  -.34
10 1  .00  .00  .01  -.02  -.01  .04  .01  .01  -.02
11 1  .00  .00  .00  -.01  -.01  .00  -.06  -.03  -.01
12 1  .00  .00  .00  -.07  .18  .10  -.03  .09  .05
13 1  .00  -.03  -.02  .01  -.06  -.05  -.12  .67  .49
14 1  .01  .01  .03  -.07  .01  .02  -.05  -.04  -.10  .24
15 1  -.04  .03  -.13  .25  -.22  .83  .01  -.01  .02
16 1  .02  .02  .06  -.01  -.01  -.02  .00  .00  .01
17 1  .00  .00  .00  .00  .00  .00  .16  -.11  .11
18 1  -.01  .00  .02  .17  .08  -.28  .05  .02  -.08
19 1  -.01  .00  .00  -.04  .02  -.02  -.01  .00  .00
20 1  .32  .18  .19  .04  .02  .02  .02  .01  .01
21 1  -.19  .33  -.80  -.02  .05  -.11  -.01  .02  -.05
      49      50      51
      ?A      ?A      ?A
Frequencies -- 3086.6155      3089.4554      3098.9384
Red. masses -- 1.0630      1.0667      1.0691
Frc consts -- 5.9672      5.9989      6.0489
IR Inten -- 23.3621      31.9360      52.8035
Raman Activ -- .0000      .0000      .0000
Depolar -- .0000      .0000      .0000
Atom AN  X   Y   Z   X   Y   Z   X   Y   Z
 1 6  .00  .00  .01  .00  .00  .00  .05  -.01  -.03

```

S107

2	6	.00	-.01	-.07	.00	.00	-.02	-.01	-.01	.00
3	6	.00	.02	.00	-.01	-.06	.02	.00	.00	.00
4	6	.00	.00	.00	.00	.01	.00	.01	-.02	-.03
5	6	.00	.00	-.01	.01	-.01	.03	.00	.00	.00
6	7	.00	.00	.00	.00	.00	.00	.00	.00	.00
7	6	.00	.00	.00	.00	.00	.00	.00	.00	.00
8	6	.00	.00	.00	.00	.00	.00	.00	.00	.00
9	1	.05	.03	-.15	-.01	-.01	.05	-.20	-.14	.64
10	1	-.35	-.16	.71	-.12	-.05	.25	-.01	.00	.02
11	1	.40	.25	.07	.07	.04	.01	.13	.08	.02
12	1	.08	-.22	-.12	-.18	.51	.28	.02	-.05	-.03
13	1	-.01	.02	.02	.01	-.06	-.04	-.05	.32	.24
14	1	.00	-.01	.01	.00	.00	.00	-.02	-.05	.12
15	1	.02	-.02	.07	-.11	.09	-.36	.01	-.01	.04
16	1	.00	.00	-.01	-.01	-.01	-.01	.00	.00	.01
17	1	.00	.00	.00	-.04	.03	-.03	-.40	.27	-.27
18	1	-.05	-.02	.09	.31	.14	-.51	.00	.00	.00
19	1	.00	.00	.00	.03	-.02	.02	-.01	.00	.00
20	1	-.01	.00	.00	.00	.00	.00	.00	.00	.00
21	1	.00	.00	.00	.01	-.02	.04	-.01	.01	-.02

52

?A

53

?A

54

?A

Frequencies -- 3119.8480 3122.3128 3135.6637

Red. masses -- 1.0939 1.0711 1.1029

Frc consts -- 6.2735 6.1522 6.3894

IR Inten -- 41.7741 28.1562 21.9465

Raman Activ -- .0000 .0000 .0000

Depolar -- .0000 .0000 .0000

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	.00	.00	.00	.00	.00	.00	.00	.00	.01
2	6	.00	.00	.00	.00	.00	.00	-.03	-.02	.00
3	6	.00	.00	.00	.00	.00	.00	.04	-.03	-.07
4	6	.00	.00	.00	.00	.00	.00	.00	.00	.00
5	6	.00	.00	.00	.00	.00	.00	.00	.00	-.01
6	7	.00	.00	.00	.00	.00	.00	.00	.00	.00
7	6	.01	-.02	-.03	-.03	.04	.03	.00	.00	.00
8	6	.06	.02	.05	.03	.01	.03	.00	.00	.00
9	1	.00	.00	-.01	.00	.00	.00	.02	.01	-.06
10	1	.00	.00	.01	.00	.00	-.01	.04	.02	-.10
11	1	-.02	-.01	.00	-.01	-.01	.00	.33	.21	.07
12	1	.01	-.01	-.01	-.01	.02	.01	-.19	.57	.29
13	1	.00	-.02	-.01	.00	.00	.00	.00	.00	.00
14	1	.00	.00	.01	.00	.00	.00	.00	.00	-.01
15	1	.00	.00	-.01	.00	.00	.01	.02	-.02	.07
16	1	.11	.19	.42	-.16	-.27	-.58	.01	.01	.03
17	1	.00	.00	.00	.00	.00	.00	-.04	.02	-.02
18	1	.02	.01	-.04	-.02	-.01	.04	-.30	-.16	.50
19	1	-.18	.08	-.09	.48	-.21	.22	-.05	.02	-.02
20	1	-.61	-.38	-.32	-.33	-.21	-.17	-.02	-.01	-.01
21	1	-.06	.13	-.28	-.05	.10	-.22	.00	.00	-.01

55

?A

56

?A

57

?A

Frequencies -- 3147.1062 3152.4284 3188.0774

Red. masses -- 1.1020 1.1053 1.1086

Frc consts -- 6.4309 6.4719 6.6386

IR Inten -- 40.4176 42.3624 31.3327

Raman Activ -- .0000 .0000 .0000

Depolar -- .0000 .0000 .0000

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-.02	.02	-.03	-.03	.04	-.07	.00	.00	.00
2	6	-.06	-.04	.02	.03	.02	-.02	.00	.00	.00
3	6	-.02	.01	.03	.01	-.01	-.02	.00	.00	.00
4	6	.00	.00	.00	.00	.00	-.01	.00	.00	.00
5	6	.00	.00	.00	.00	.00	.00	.00	.00	-.01
6	7	.00	.00	.00	.00	.00	.00	.00	.00	.00
7	6	.00	.00	.00	.00	.00	.00	-.07	.01	-.07
8	6	.00	.00	.00	.00	.00	.00	-.01	.00	-.01
9	1	-.07	-.04	.18	-.18	-.10	.52	.00	.00	.01
10	1	.16	.07	-.35	-.13	-.05	.27	-.01	.00	.02
11	1	.58	.37	.12	-.25	-.16	-.05	-.01	-.01	.00
12	1	.05	-.15	-.08	-.04	.12	.06	-.01	.02	.01

S108

13	1	.00	.00	.00	-.01	.03	.02	.00	.00	.00
14	1	.00	-.01	.02	-.01	-.03	.07	.00	.00	.00
15	1	-.01	.01	-.03	.01	-.01	.02	.02	-.02	.06
16	1	.00	.00	.00	.00	.00	.00	.12	.25	.51
17	1	.34	-.22	.21	.49	-.32	.30	.00	.00	.00
18	1	.14	.07	-.23	-.10	-.06	.17	-.01	-.01	.02
19	1	.03	-.01	.01	-.02	.01	-.01	.67	-.32	.28
20	1	-.01	.00	.00	.00	.00	.00	.08	.05	.04
21	1	.00	.00	.00	.00	.00	.00	.01	-.03	.06

- Thermochemistry -

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Atom 1 has atomic number 6 and mass 12.00000

Atom 2 has atomic number 6 and mass 12.00000

Atom 3 has atomic number 6 and mass 12.00000

Atom 4 has atomic number 6 and mass 12.00000

Atom 5 has atomic number 6 and mass 12.00000

Atom 6 has atomic number 7 and mass 14.00307

Atom 7 has atomic number 6 and mass 12.00000

Atom 8 has atomic number 6 and mass 12.00000

Atom 9 has atomic number 1 and mass 1.00783

Atom 10 has atomic number 1 and mass 1.00783

Atom 11 has atomic number 1 and mass 1.00783

Atom 12 has atomic number 1 and mass 1.00783

Atom 13 has atomic number 1 and mass 1.00783

Atom 14 has atomic number 1 and mass 1.00783

Atom 15 has atomic number 1 and mass 1.00783

Atom 16 has atomic number 1 and mass 1.00783

Atom 17 has atomic number 1 and mass 1.00783

Atom 18 has atomic number 1 and mass 1.00783

Atom 19 has atomic number 1 and mass 1.00783

Atom 20 has atomic number 1 and mass 1.00783

Atom 21 has atomic number 1 and mass 1.00783

Molecular mass: 111.10480 amu.

Principal axes and moments of inertia in atomic units:

	1	2	3
EIGENVALUES --	550.34325	855.36213	1180.74429
X	.99994	-.00950	-.00615
Y	.00940	.99983	-.01586
Z	.00630	.01580	.99986

THIS MOLECULE IS AN ASYMMETRIC TOP.

ROTATIONAL SYMMETRY NUMBER 1.

WARNING-- ASSUMPTION OF CLASSICAL BEHAVIOR FOR ROTATION
MAY CAUSE SIGNIFICANT ERROR

ROTATIONAL TEMPERATURES (KELVIN) .15738 .10126 .07335

ROTATIONAL CONSTANTS (GHZ) 3.27930 2.10991 1.52848

1 IMAGINARY FREQUENCIES IGNORED.

Zero-point vibrational energy 519218.0 (Joules/Mol)

124.09607 (Kcal/Mol)

WARNING-- EXPLICIT CONSIDERATION OF 6 DEGREES OF FREEDOM AS
VIBRATIONS MAY CAUSE SIGNIFICANT ERRORVIBRATIONAL TEMPERATURES: 146.50 420.48 504.47 553.29 619.52
(KELVIN) 687.59 897.56 929.43 1089.55 1175.14

1222.81	1294.45	1306.97	1379.89	1416.89
1461.92	1507.70	1519.26	1562.15	1584.67
1671.29	1674.57	1708.72	1742.51	1778.76
1807.68	1861.90	1869.20	1879.58	1897.17
1939.28	1969.20	1999.17	2033.23	2051.28
2062.29	2074.02	2221.43	2225.23	2236.93
2247.67	2268.10	2295.51	4353.64	4400.15
4420.21	4437.80	4440.93	4445.01	4458.66
4488.74	4492.29	4511.49	4527.96	4535.62
4586.91				

Zero-point correction=.197760 (Hartree/Particle)

Thermal correction to Energy=.204028

Thermal correction to Enthalpy=.204972

Thermal correction to Gibbs Free Energy=.167312

Sum of electronic and zero-point Energies=-327.921931

S109

Sum of electronic and thermal Energies= -327.915663
 Sum of electronic and thermal Enthalpies= -327.914719
 Sum of electronic and thermal Free Energies= -327.952379

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	128.030	25.509	79.263
ELECTRONIC	.000	.000	.000
TRANSLATIONAL	.889	2.981	40.032
ROTATIONAL	.889	2.981	27.810
VIBRATIONAL	126.252	19.547	11.421
VIBRATION 1	.604	1.948	3.419
VIBRATION 2	.688	1.688	1.461
VIBRATION 3	.728	1.574	1.163
VIBRATION 4	.754	1.503	1.021
VIBRATION 5	.792	1.404	.857
VIBRATION 6	.834	1.299	.716
Q	LOG10(Q)	LN(Q)	
TOTAL BOT	.110248D-76	-76.957630	-177.201491
TOTAL V=0	.101133D+15	14.004892	32.247456
VIB (BOT)	.897411D-90	-90.047009	-207.340900
VIB (BOT) 1	.201476D+01	.304224	.700501
VIB (BOT) 2	.653545D+00	-.184724	-.425344
VIB (BOT) 3	.525989D+00	-.279023	-.642474
VIB (BOT) 4	.468659D+00	-.329143	-.757880
VIB (BOT) 5	.404471D+00	-.393113	-.905176
VIB (BOT) 6	.350590D+00	-.455201	-1.048139
VIB (V=0)	.823215D+01	.915513	2.108047
VIB (V=0) 1	.257588D+01	.410925	.946190
VIB (V=0) 2	.132287D+01	.121518	.279807
VIB (V=0) 3	.122572D+01	.088390	.203526
VIB (V=0) 4	.118530D+01	.073830	.169999
VIB (V=0) 5	.114311D+01	.058090	.133757
VIB (V=0) 6	.111067D+01	.045584	.104960
ELECTRONIC	.100000D+01	.000000	.000000
TRANSLATIONAL	.460320D+08	7.663060	17.644847
ROTATIONAL	.266882D+06	5.426319	12.494562

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr)		
		X	Y	Z
1	6	-.000010221	.000004984	.000004038
2	6	-.000003911	-.000001021	.000002897
3	6	.000003016	-.000005910	-.000002872
4	6	-.000003724	-.000016125	.000033193
5	6	-.000002244	.000014916	.000011996
6	7	.000003902	-.000016448	-.000036406
7	6	.000020703	-.000009253	.000002581
8	6	-.000015462	.000008761	.000005432
9	1	.000005922	.000009099	-.000020910
10	1	.000000529	-.000001302	.000001535
11	1	-.000000794	-.000002424	-.000002155
12	1	-.000001933	.000000455	.000002779
13	1	-.000006519	.000018068	.000006649
14	1	.000005788	.000002058	-.000016823
15	1	-.000001821	-.000000700	-.000002370
16	1	-.000003847	.000004296	-.000000010
17	1	.000015934	-.000009060	.000010020
18	1	.000000095	.000001414	-.000001218
19	1	-.000007752	.000002840	-.000006279
20	1	-.000001256	-.000003435	.000000371
21	1	.000003594	-.000001212	.000007551

Cartesian Forces: Max .000036406 RMS .000010109
 1\1\GINC-ARMON\Freq\RMP2-FC\6-31G(d)\C7H13N1\BELOSTOT\22-Oct-2002\0\#\n
 MP2/6-31G* OPT=(CARTESIAN, NEWTON, TS, CALCALL) GEOM=ALLCHECKPOINT GU
 ESS=CHECKPOINT\1-Azabicyclo420octane, 4-sofa transition state\0,1\C,
 1.8769097424,-0.5528791911,-0.0663417311\C,1.5252970663,0.7549796848,0
 .6360946521\C,0.5595781208,1.529783027,-0.2549431168\C,0.661212214,-1.
 4734314017,-0.0839137932\C,-0.6603064821,0.6886221087,-0.6392847029\N,

S110

-0.5585421541,-0.8045679506,-0.5375973989\C,-1.8523975584,0.6739493886
,0.3413698233\C,-1.7291028188,-0.8600145799,0.3644935485\H,2.205419523
7,-0.3344575218,-1.090477716\H,1.0702965367,0.5377550756,1.6123337612\
H,2.4223106075,1.354385423,0.8289061468\H,0.217106776,2.4573756853,0.2
220140403\H,0.8615731232,-2.3549033282,-0.7092244993\H,0.5106714633,-1
.8463403026,0.9433414001\H,-0.9750859457,0.9623229114,-1.6556903858\H,
-1.6265755335,1.1459343559,1.3028981735\H,2.7052559574,-1.0710381355,0
.4304310794\H,1.1042185804,1.8257724642,-1.1603035457\H,-2.789675764,1
.0871206776,-0.0407573476\H,-2.5775181494,-1.4117692258,-0.0590430514\
H,-1.5053438022,-1.2862366439,1.3539056571\\Version=IBM-RS6000-G98RevA
.7\HF=-327.0460199\MP2=-328.1196909\RMSD=1.560e-09\RMSF=1.011e-05\Dipo
le=0.1439043,0.2905153,0.3746308\

Conformation 8 (RI transition state)

Item Value Threshold Converged?
 Maximum Force .000025 .000450 YES
 RMS Force .000009 .000300 YES
 Maximum Displacement .001279 .001800 YES
 RMS Displacement .000389 .001200 YES
 Predicted change in Energy=-6.220201D-09

Optimization completed.

-- Stationary point found.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.481182	-.962581	-.859769
2	6	0	-1.484759	-.933377	.665734
3	6	0	-.052166	-.966827	1.228028
4	6	0	-.845854	.321543	-1.380048
5	6	0	1.000399	-.410282	.240295
6	7	0	.497055	.496226	-.826320
7	6	0	1.812205	.789641	.775428
8	6	0	.819654	1.671978	-.002319
9	1	0	-.917609	-1.831660	-1.222851
10	1	0	-1.990086	-.012425	.984075
11	1	0	-2.069076	-1.764714	1.075232
12	1	0	-.013351	-.416384	2.175455
13	1	0	-.802795	.321211	-2.477631
14	1	0	-1.481946	1.171089	-1.082685
15	1	0	1.594357	-1.235960	-.172192
16	1	0	1.859735	.910302	1.860603
17	1	0	-2.499935	-1.054683	-1.253382
18	1	0	.221910	-2.000868	1.467708
19	1	0	2.818120	.833743	.352862
20	1	0	1.212574	2.534058	-.554516
21	1	0	-.021067	2.012141	.627467

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.898530	-.425381	-.272581
2	6	0	1.593475	.823149	.549696
3	6	0	.323464	1.529426	.041897
4	6	0	.789723	-1.448056	-.053512
5	6	0	-.651202	.574734	-.687378
6	7	0	-.515828	-.874594	-.380942
7	6	0	-2.062758	.499682	-.065215
8	6	0	-1.566884	-.773015	.643952
9	1	0	1.967625	-.172164	-1.338342
10	1	0	1.457298	.514002	1.594077
11	1	0	2.439896	1.518650	.540394
12	1	0	-.183828	2.025248	.877916
13	1	0	.964822	-2.351192	-.653702
14	1	0	.803384	-1.756511	1.004522
15	1	0	-.620824	.768388	-1.767309
16	1	0	-2.374307	1.341936	.557655
17	1	0	2.862306	-.860198	.016108
18	1	0	.603509	2.326116	-.657148
19	1	0	-2.833898	.281611	-.806944
20	1	0	-2.244694	-1.633017	.702766
21	1	0	-1.176581	-.563952	1.655441

Rotational constants (GHZ): 3.4275203 2.0487859 1.5305049

Isotopes: C-12,C-12,C-12,C-12,C-12,N-14,C-12,C-12,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1

Rotating electric field derivatives to standard orientation.

Rotating nuclear coordinate derivatives to standard orientation.

S112

Full mass-weighted force constant matrix:

Low frequencies --- -85.8005 -1.6397 -.9072 .0010 .0010 .0011

Low frequencies --- 1.4645 141.3140 280.3520

***** 1 imaginary frequencies (negative Signs) *****

Harmonic frequencies (cm⁻¹), IR intensities (KM/Mole),Raman scattering activities (A⁴/AMU), Raman depolarization ratios,

reduced masses (AMU), force constants (mDyne/A) and normal coordinates:

1 ?A				2 ?A				3 ?A			
Frequencies --	-85.8004				141.3140				280.3520		
Red. masses --	1.9509				2.1169				2.0270		
Frc consts --	.0085				.0249				.0939		
IR Inten --	.0881				.3427				1.7340		
Raman Activ --	.0000				.0000				.0000		
Depolar --	.0000				.0000				.0000		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z		
1 6	.01	.02	.07	-.01	.01	-.03	.05	-.07	.16		
2 6	-.11	-.04	.11	-.03	-.04	.04	.04	.07	-.06		
3 6	.04	.03	-.15	-.07	-.05	.09	-.05	-.02	.01		
4 6	.01	-.02	-.11	.01	-.03	-.09	-.05	.00	-.04		
5 6	-.03	.00	-.03	.02	-.03	-.05	-.05	.02	-.04		
6 7	.00	.00	-.02	-.01	-.01	.03	-.04	-.01	-.14		
7 6	.02	.01	.08	-.01	-.02	-.12	-.01	.00	.07		
8 6	.07	.01	.05	.09	.16	.13	.09	.01	.00		
9 1	.12	.09	.10	-.02	.08	-.01	.35	-.20	.15		
10 1	-.36	-.11	.06	-.01	-.10	.03	.20	.27	.02		
11 1	-.09	-.06	.34	-.05	-.02	.07	.03	.09	-.31		
12 1	.04	.30	-.31	-.12	-.20	.15	-.06	-.16	.09		
13 1	.03	.07	-.24	.00	.04	-.20	.01	.02	-.06		
14 1	-.01	-.18	-.16	.05	-.15	-.13	-.21	-.07	-.05		
15 1	-.13	-.03	-.04	.13	-.04	-.05	-.10	.09	-.02		
16 1	.07	.01	.10	-.14	.08	-.31	.04	-.01	.10		
17 1	-.01	.01	.14	.00	.02	-.06	-.06	-.12	.45		
18 1	.24	-.18	-.30	-.11	.06	.21	-.17	.09	.10		
19 1	-.04	.00	.14	.07	-.27	-.13	-.07	-.01	.13		
20 1	.07	.01	.10	.14	.15	.40	.10	.01	.13		
21 1	.13	.02	.03	.19	.42	.03	.25	.04	-.07		

4 ?A				5 ?A				6 ?A			
Frequencies --	348.7275				377.1152				440.8448		
Red. masses --	2.1866				2.2555				3.0402		
Frc consts --	.1567				.1890				.3481		
IR Inten --	3.8352				.1311				1.8473		
Raman Activ --	.0000				.0000				.0000		
Depolar --	.0000				.0000				.0000		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z		
1 6	-.08	.03	-.05	.00	-.09	-.02	-.02	.12	.02		
2 6	-.06	-.04	.06	.01	-.07	-.02	.20	.07	.12		
3 6	-.02	-.04	.02	.06	.09	.00	.15	-.08	.00		
4 6	-.02	.04	.13	-.04	.02	.06	-.05	.10	-.04		
5 6	.01	-.01	-.06	-.05	.14	.06	-.02	-.06	.05		
6 7	-.01	-.07	-.16	.04	.10	-.03	-.15	-.11	-.09		
7 6	.07	.04	.06	-.11	-.14	-.04	-.07	-.05	-.03		
8 6	.12	.03	-.03	.09	-.02	.00	-.07	-.01	.03		
9 1	-.30	.07	-.06	.01	-.13	-.03	-.13	.27	.05		
10 1	-.10	-.14	.02	-.06	-.11	-.04	.32	.16	.16		
11 1	-.06	-.03	.16	.05	-.12	.06	.17	.10	-.07		
12 1	-.08	-.06	.00	.17	.21	-.01	.17	.20	-.16		
13 1	.04	-.15	.44	-.13	-.09	.19	.08	.13	-.05		
14 1	-.09	.38	.24	-.10	.17	.10	-.06	.07	-.05		
15 1	-.03	.06	-.05	-.09	.19	.07	-.02	.00	.06		
16 1	.19	.04	.10	-.44	-.21	-.11	-.22	-.05	-.11		
17 1	-.01	.07	-.24	-.01	-.09	.02	-.03	-.05	-.18		
18 1	.02	-.02	.06	.17	.00	-.06	.24	-.29	-.21		
19 1	-.03	.08	.15	.08	-.37	-.17	.06	-.16	-.13		
20 1	.10	.06	.13	.25	-.13	.12	-.07	.01	.21		
21 1	.33	.04	-.11	.14	.13	-.05	.07	.11	-.05		

7 ?A				8 ?A				9 ?A			
Frequencies --	460.5159				627.0813				667.1184		
Red. masses --	2.9751				2.5287				2.6067		

S113

Frc consts --	.3717	.5859	.6835
IR Inten --	.3131	6.3439	2.8265
Raman Activ --	.0000	.0000	.0000
Depolar --	.0000	.0000	.0000

Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	.24	.01	-.05	.06	.01	-.06	.05	-.03	.03
2 6	.03	-.11	.00	-.07	.03	-.09	.00	-.01	.01
3 6	-.02	-.17	-.02	.00	.14	.05	-.02	.00	.02
4 6	.08	.16	.02	.04	-.03	-.02	.17	-.17	.06
5 6	-.12	-.02	-.05	.06	-.01	.16	-.11	.05	.06
6 7	-.02	.04	.01	-.08	-.17	-.09	.07	-.07	-.05
7 6	-.11	.04	.02	.04	.02	-.01	-.15	.07	.00
8 6	-.07	.04	.01	-.08	.02	.03	-.02	.10	-.09
9 1	.46	-.01	-.04	.41	-.17	-.08	-.30	.02	.01
10 1	-.10	-.31	-.07	-.27	-.18	-.18	.15	.12	.07
11 1	-.10	.04	.27	-.02	-.02	.23	-.03	.03	-.18
12 1	.02	-.21	.03	.11	.22	.07	.07	.19	-.04
13 1	.00	.03	.21	.09	-.12	.13	.19	-.07	-.08
14 1	.13	.38	.08	.11	.14	.03	.12	-.31	.01
15 1	-.15	.00	-.05	.12	.03	.17	-.15	.12	.07
16 1	-.03	.05	.05	-.09	.03	-.08	-.06	.00	.16
17 1	.13	-.09	.16	-.03	.05	.34	.23	.19	-.26
18 1	-.01	-.11	.05	-.08	.05	-.08	.07	-.12	-.09
19 1	-.18	.08	.08	.19	.00	-.16	-.20	.23	.00
20 1	-.06	.03	-.01	-.18	.10	.18	.03	.07	.12
21 1	-.10	.05	.02	.06	.08	-.04	-.02	.32	-.13

10 11 12
?A ?A ?A

Frequencies --	777.4613	798.7830	867.6627
Red. masses --	1.8631	1.3710	1.7758
Frc consts --	.6635	.5154	.7877
IR Inten --	.9375	1.7851	.3459
Raman Activ --	.0000	.0000	.0000
Depolar --	.0000	.0000	.0000

Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	-.03	.01	-.01	-.03	.01	-.03	.05	-.05	-.06
2 6	-.10	-.03	-.02	.02	.02	.00	.01	-.01	.11
3 6	-.08	-.14	.05	.01	.04	.03	-.06	.13	.07
4 6	-.01	.04	-.03	-.05	.03	-.02	.02	-.05	-.06
5 6	.01	-.02	.13	.04	-.08	.02	-.03	.01	-.11
6 7	.05	.05	.01	.01	.01	.05	-.01	-.01	.01
7 6	.06	.05	-.02	-.08	-.02	-.05	.01	-.03	-.02
8 6	.05	.01	-.04	.03	-.02	-.06	-.02	-.01	.06
9 1	.13	.01	.00	.15	-.03	-.02	.21	.11	-.01
10 1	.27	.09	.06	-.02	-.06	-.02	.36	.11	.18
11 1	-.20	.08	-.39	.06	-.03	.07	.02	-.02	-.26
12 1	.04	.34	-.17	.02	.09	.01	-.15	.37	-.12
13 1	-.06	-.01	.04	-.07	.01	.00	-.12	-.27	.23
14 1	.02	.13	.00	.02	.06	-.01	.11	.29	.04
15 1	.06	.05	.15	.19	-.15	.01	.06	-.01	-.11
16 1	-.01	.06	-.08	.32	-.13	.29	.17	.06	-.06
17 1	-.07	.04	.15	-.12	-.08	.13	.02	-.07	.03
18 1	.13	-.49	-.27	-.01	-.02	-.04	.23	-.05	-.02
19 1	.18	.03	-.14	-.30	.42	.06	-.18	-.07	.18
20 1	.05	.00	-.06	.28	-.19	.24	-.10	.04	-.07
21 1	.04	-.01	-.03	.02	.39	-.13	-.06	-.13	.10

13 14 15
?A ?A ?A

Frequencies --	902.5099	947.2261	955.1618
Red. masses --	2.1725	1.7972	1.6215
Frc consts --	1.0426	.9501	.8716
IR Inten --	2.4941	1.2506	.0338
Raman Activ --	.0000	.0000	.0000
Depolar --	.0000	.0000	.0000

Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	.16	-.08	-.05	.09	-.02	.02	.03	-.02	.02
2 6	.08	.13	.07	-.05	-.03	.01	.02	-.04	-.06
3 6	-.11	.00	-.02	-.02	-.02	-.05	-.04	.04	.08
4 6	-.10	-.07	.00	-.01	.01	-.01	.01	.10	.08
5 6	.01	-.06	.07	.02	.10	.01	-.05	.02	-.04
6 7	-.02	.06	-.01	-.05	.02	-.01	-.04	-.01	-.03

S114

7	6	.01	.04	-.01	.13	-.09	-.03	.05	-.02	-.07
8	6	.04	-.01	-.02	-.10	-.05	.05	.00	-.05	.06
9	1	-.16	-.06	-.07	-.12	.17	.05	-.21	-.31	-.06
10	1	-.17	.00	.00	.04	.17	.08	.07	-.24	-.11
11	1	-.06	.30	.38	-.14	.06	-.18	-.04	.03	.07
12	1	-.13	.11	-.09	-.04	-.12	.00	.10	.33	.01
13	1	-.29	-.11	.01	-.09	-.04	.03	.15	.36	-.27
14	1	-.23	-.09	.00	-.05	.06	.00	-.14	-.34	-.05
15	1	.05	-.06	.08	-.15	.15	.01	.08	.07	-.03
16	1	-.01	.07	-.08	.20	-.24	.21	.31	.12	-.12
17	1	.23	-.16	-.37	.18	.05	-.20	.07	.01	-.08
18	1	-.27	-.10	-.20	.03	.08	.08	.13	-.16	-.08
19	1	.08	.00	-.07	.19	.31	-.19	-.13	.05	.10
20	1	.07	-.04	-.03	.04	-.14	.36	.02	-.07	.01
21	1	.11	-.06	-.04	-.12	.39	-.03	.01	-.08	.06

16

17

18

?A

?A

?A

Frequencies --	984.1322	996.5948	1013.3773
Red. masses --	2.0314	2.2259	2.1660
Frc consts --	1.1592	1.3026	1.3105
IR Inten --	.5051	2.1156	3.2208
Raman Activ --	.0000	.0000	.0000
Depolar --	.0000	.0000	.0000

Atom AN		X			Y			Z		
1	6	-.02	-.05	.05	-.06	-.09	.00	.08	-.05	.07
2	6	.01	-.08	.02	.08	-.04	.05	-.09	-.08	-.04
3	6	-.02	.08	-.06	-.11	.07	-.03	.00	.06	-.01
4	6	.05	.07	-.05	.03	.13	-.02	.02	.10	-.02
5	6	-.07	-.04	.08	-.05	-.03	.04	.15	-.10	.03
6	7	.00	-.02	.00	.08	-.05	.02	-.01	.04	-.07
7	6	-.03	.14	-.08	.10	-.08	.04	-.08	-.04	.06
8	6	.05	-.12	.06	-.03	.11	-.09	-.04	.07	.00
9	1	-.10	.22	.11	-.04	-.08	.00	-.26	.16	.09
10	1	-.07	.19	.09	.01	-.03	.05	-.04	.21	.05
11	1	.14	-.24	-.14	.16	-.13	.06	-.04	-.14	-.26
12	1	.04	-.11	.08	-.17	.07	-.07	.05	.03	.04
13	1	.08	.00	.06	.17	.20	-.09	-.03	.10	-.03
14	1	.11	.20	-.01	.13	.03	-.05	-.14	.06	-.04
15	1	-.11	-.08	.07	-.28	.00	.04	.49	-.22	.02
16	1	.05	.34	-.29	-.02	-.20	.14	-.09	-.08	.11
17	1	-.01	-.19	-.16	-.21	-.48	-.08	.23	.05	-.29
18	1	-.21	.20	.00	-.20	.04	-.10	-.08	.05	-.05
19	1	.07	.21	-.20	.17	-.07	-.03	-.19	-.19	.21
20	1	.21	-.25	.08	-.23	.28	-.03	-.11	.12	-.08
21	1	.13	-.13	.03	-.09	.20	-.09	.03	-.08	.00

19

20

21

?A

?A

?A

Frequencies --	1064.2420			1089.0034			1116.4598		
Red. masses --	1.7413			2.7411			1.6471		
Frc consts --	1.1620			1.9153			1.2097		
IR Inten --	7.3145			9.1762			10.4744		
Raman Activ --	.0000			.0000			.0000		
Depolar --	.0000			.0000			.0000		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	-.03	.01	.06	.11	.11	.03	.01	-.07	-.02
2 6	.02	.03	-.05	-.01	-.11	-.04	-.07	.06	.01
3 6	.04	-.03	.03	.01	.08	.01	.05	-.05	.00
4 6	.00	-.04	-.07	-.13	-.01	.04	-.01	.04	-.01
5 6	-.09	-.05	.06	-.12	-.03	.03	-.01	.11	.02
6 7	.07	.06	-.05	-.07	-.08	.12	-.03	-.10	.05
7 6	.04	-.10	-.06	.07	-.02	-.03	-.01	-.01	-.06
8 6	-.03	.06	.05	.12	.04	-.15	.07	.02	-.01
9 1	-.08	.13	.08	.10	.44	.10	-.03	.04	.01
10 1	-.25	.06	-.07	.09	.00	.00	-.20	.31	.06
11 1	.12	-.09	.14	.02	-.15	-.18	-.30	.34	.00
12 1	.31	.02	.16	.23	.03	.17	.26	-.05	.13
13 1	.00	-.21	.18	-.32	.03	-.07	.06	.05	-.01
14 1	-.17	.21	.01	-.04	-.14	.01	.23	.05	-.01
15 1	-.12	.17	.09	-.21	-.15	.01	.20	.09	.02
16 1	.46	.11	-.14	.09	-.05	.00	.11	-.06	.07
17 1	.03	.12	-.02	.21	.28	-.03	-.11	-.46	-.18

S115

18	1	-0.19	-0.07	-0.11	.01	.12	.04	.05	.00	.05
19	1	-.21	-.03	.18	.04	-.11	.04	-.20	-.03	.14
20	1	-.13	.14	-.11	-.11	.22	-.14	-.05	.10	-.17
21	1	-.15	.00	.10	.17	-.06	-.15	-.06	-.11	.07
	22				23			24		
	?A				?A			?A		
Frequencies --		1151.1553			1175.5225			1185.3577		
Red. masses --		2.0145			1.2745			2.0145		
Frc consts --		1.5728			1.0377			1.6677		
IR Inten --		3.4886			.9917			6.2632		
Raman Activ --		.0000			.0000			.0000		
Depolar --		.0000			.0000			.0000		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z	
1	6	-.02	.06	.05	-.02	.02	-.02	-.01	-.04	.09
2	6	.12	-.07	-.04	.02	-.01	.02	.01	.04	-.09
3	6	-.14	-.04	-.05	-.02	-.02	-.04	-.01	-.02	.12
4	6	.00	-.05	.00	.01	-.02	.04	.03	.00	-.09
5	6	.05	.15	.01	.01	.06	.02	-.03	-.01	-.14
6	7	-.07	-.03	.00	.02	.06	.00	-.01	.01	.09
7	6	.00	.00	-.03	-.01	-.02	-.02	.04	.07	.05
8	6	.06	.01	.04	-.06	-.06	-.03	-.03	-.07	-.06
9	1	.06	.27	.11	.11	.10	.01	-.18	.08	.11
10	1	-.08	-.13	-.08	-.02	.03	.03	-.27	.04	-.13
11	1	.23	-.21	.10	.03	-.02	.00	.07	-.03	.15
12	1	-.06	.09	-.08	.01	-.04	-.01	.23	.27	.10
13	1	.11	-.07	.07	-.09	.04	-.07	.11	-.13	.14
14	1	.09	.06	.03	.23	-.11	.02	.03	.25	-.01
15	1	.42	.05	.01	.20	.02	.02	.09	-.04	-.15
16	1	-.06	-.21	.23	.14	.10	-.10	-.33	-.13	.13
17	1	-.02	.05	.02	-.07	-.05	.05	.06	-.06	-.16
18	1	-.33	-.16	-.26	-.11	-.01	-.05	.03	-.22	-.09
19	1	-.09	.04	.05	-.16	-.09	.16	.20	-.05	-.08
20	1	.11	-.05	-.22	-.38	.21	.41	-.12	.02	.29
21	1	-.21	-.06	.16	.52	-.13	-.24	.20	.08	-.17
	25				26			27		
	?A				?A			?A		
Frequencies --		1214.7395			1232.1003			1271.3607		
Red. masses --		1.5233			1.5053			1.6907		
Frc consts --		1.3244			1.3464			1.6101		
IR Inten --		12.0942			3.7805			12.7925		
Raman Activ --		.0000			.0000			.0000		
Depolar --		.0000			.0000			.0000		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z	
1	6	.02	.05	.04	.01	.06	.01	.01	.01	-.04
2	6	.02	-.04	-.02	.02	-.05	-.03	-.01	.00	-.02
3	6	-.03	.02	-.04	-.05	.02	-.01	.00	.00	.06
4	6	-.07	.00	-.07	-.07	-.04	.02	-.07	.01	.08
5	6	.01	.03	.03	.03	.02	-.03	.02	-.04	-.07
6	7	.11	-.05	.03	.08	-.03	-.02	.12	-.03	-.07
7	6	-.05	.02	-.05	.00	.00	.10	-.04	.02	-.03
8	6	.01	-.02	.05	-.07	-.01	-.03	-.02	.01	.11
9	1	-.10	-.07	.00	.12	.30	.07	.20	.36	.05
10	1	.22	-.26	-.06	.03	-.05	-.03	-.20	.20	.01
11	1	-.19	.22	.03	-.19	.21	.01	.07	-.10	-.02
12	1	-.07	-.05	-.03	.21	.07	.12	.11	.11	.05
13	1	.32	-.09	.14	.12	.01	.00	-.31	.10	-.13
14	1	-.47	.11	-.03	-.04	-.07	.01	.10	-.24	.01
15	1	-.01	-.09	.01	.08	.03	-.02	-.17	.16	-.04
16	1	-.07	-.12	.14	.06	.35	-.34	-.20	-.22	.23
17	1	-.01	-.06	-.06	-.14	-.33	-.08	-.07	-.16	-.02
18	1	.21	.08	.12	.03	.01	.01	-.05	-.09	-.07
19	1	-.06	.18	-.09	.04	-.21	.12	.06	.29	-.22
20	1	-.30	.22	.10	.24	-.24	.07	-.09	.06	-.02
21	1	.13	-.16	.04	-.20	.28	-.04	.03	-.20	.13
	28				29			30		
	?A				?A			?A		
Frequencies --		1282.4028			1296.0798			1301.2105		
Red. masses --		1.4887			1.6126			1.4055		
Frc consts --		1.4425			1.5960			1.4021		
IR Inten --		7.5228			7.1468			6.1521		
Raman Activ --		.0000			.0000			.0000		

S116

Depolar	--	.0000			.0000			.0000		
Atom AN		X	Y	Z	X	Y	Z	X	Y	Z
1	6	-.03	.03	-.05	.02	-.02	-.04	.00	-.02	-.01
2	6	.00	-.03	.07	-.02	.02	.04	.00	.03	.02
3	6	.00	.03	-.03	.03	-.02	.00	.00	-.03	.00
4	6	.05	-.04	.03	-.05	.05	-.01	-.02	.04	-.01
5	6	-.10	-.04	-.01	-.03	.04	.01	-.06	.07	-.02
6	7	-.02	.07	-.05	.10	-.08	.01	.05	-.04	-.02
7	6	.06	.04	-.02	.06	.11	-.04	-.04	-.06	.09
8	6	.00	-.01	.03	-.03	-.07	.00	.06	-.04	.00
9	1	.10	-.09	-.06	-.01	-.14	-.07	-.04	-.09	-.03
10	1	.14	.01	.10	-.06	.13	.07	-.06	.06	.02
11	1	-.17	.18	-.04	.15	-.19	-.06	.12	-.11	.01
12	1	.49	.01	.27	-.07	-.05	-.05	.03	.00	.00
13	1	.12	-.01	.00	-.13	.04	-.03	-.24	.02	-.04
14	1	-.13	-.08	.02	-.25	-.02	-.04	-.01	.01	-.02
15	1	.31	-.40	-.06	.10	.10	.03	.41	-.31	-.07
16	1	-.16	-.23	.22	-.21	-.10	.11	.10	.24	-.23
17	1	-.11	-.08	.07	.10	.25	.07	.08	.20	.04
18	1	-.22	.08	-.06	-.16	-.02	-.07	.03	-.01	.03
19	1	.11	-.04	-.03	-.23	-.42	.41	.22	.27	-.28
20	1	-.03	.01	.00	.00	-.08	.15	-.26	.22	.02
21	1	-.08	.05	.05	-.23	.26	.02	-.25	.18	.07

31

32

33

?A

?A

?A

Frequencies --	1319.5411	1338.5987	1362.7716
Red. masses --	1.2866	1.3001	1.5002
Frc consts --	1.3199	1.3726	1.6415
IR Inten --	6.6811	5.7842	7.0365
Raman Activ --	.0000	.0000	.0000
Depolar --	.0000	.0000	.0000

Atom AN		X	Y	Z	X	Y	Z	X	Y	Z
1	6	.03	.02	-.08	-.01	-.01	.02	-.01	.01	.03
2	6	-.03	-.01	.04	.01	-.02	.06	-.01	-.02	-.01
3	6	.02	-.01	.02	-.02	.01	-.04	.02	.03	.01
4	6	.00	-.01	.02	-.02	.04	-.04	.04	-.01	.02
5	6	.03	.01	-.04	.06	.01	-.05	.07	-.05	-.02
6	7	-.04	.01	.06	.02	-.06	.04	-.05	.04	-.02
7	6	-.03	-.03	.03	-.03	-.02	.02	-.03	.03	-.01
8	6	.03	-.01	-.02	-.03	.03	.00	.11	-.11	.00
9	1	.15	-.03	-.09	-.16	-.29	-.06	-.02	.08	.05
10	1	-.14	.27	.11	.21	-.11	.07	.16	-.17	-.04
11	1	.12	-.21	-.13	-.12	.13	.00	-.16	.16	.01
12	1	.03	.03	.01	.41	.04	.21	-.03	.00	-.01
13	1	.51	.04	.06	-.21	-.02	.00	-.17	-.01	-.03
14	1	-.50	-.09	.00	.14	.09	-.03	.08	.02	.02
15	1	-.05	.26	.00	-.07	.35	.00	-.24	.29	.03
16	1	.06	.10	-.09	.01	.04	-.03	-.06	.04	-.02
17	1	-.03	-.07	.00	.09	.28	.11	-.05	-.11	-.01
18	1	-.28	-.06	-.16	-.37	.01	-.18	-.20	.00	-.12
19	1	.06	.11	-.11	.04	.10	-.09	-.07	-.04	.05
20	1	-.07	.07	.03	.10	-.07	-.01	-.42	.31	.08
21	1	.03	-.01	-.02	.15	-.14	-.03	-.40	.35	.10

34

35

36

?A

?A

?A

Frequencies --	1383.4554	1404.9086	1419.8899
Red. masses --	1.3198	1.4626	1.4267
Frc consts --	1.4882	1.7009	1.6947
IR Inten --	3.4569	3.2895	1.2328
Raman Activ --	.0000	.0000	.0000
Depolar --	.0000	.0000	.0000

Atom AN		X	Y	Z	X	Y	Z	X	Y	Z
1	6	-.02	-.07	-.01	-.05	-.05	-.04	.07	.13	.03
2	6	.03	-.06	-.02	.10	-.04	.01	-.01	-.04	.01
3	6	.09	.02	.07	-.12	.00	-.03	-.01	-.01	.03
4	6	-.06	.01	.00	.00	.01	.00	-.07	-.04	-.02
5	6	.00	.04	-.01	.07	-.02	.01	.05	.03	.00
6	7	.02	.01	-.01	-.02	.01	.00	.01	.02	-.03
7	6	.00	-.01	.00	-.02	.01	-.01	-.01	.00	-.01
8	6	-.01	.01	.01	.02	-.02	.00	.01	-.01	.01
9	1	.02	.16	.05	.08	.00	-.02	-.21	-.55	-.15

S117

10	1	-.04	.10	.02	-.35	.40	.08	-.14	.22	.07
11	1	-.29	.33	.06	-.07	.16	.09	.11	-.19	-.10
12	1	-.28	.02	-.15	.27	.07	.17	.04	.02	.04
13	1	.28	.08	-.01	.10	.06	-.03	.05	-.03	-.01
14	1	.18	.03	.01	-.05	.03	.00	.35	.10	.02
15	1	-.17	-.37	-.08	-.26	-.06	.00	-.31	-.36	-.07
16	1	.00	.02	-.04	.00	.01	.01	-.01	.01	-.02
17	1	.11	.31	.10	.09	.38	.13	-.07	-.23	-.05
18	1	-.40	-.06	-.22	.43	.01	.21	-.05	-.08	-.06
19	1	-.02	.03	.01	-.05	-.05	.04	-.07	.00	.05
20	1	.02	-.02	.00	-.09	.06	.02	-.04	.03	.02
21	1	.01	-.02	.00	-.07	.07	.02	-.06	.03	.03

37

38

39

?A

?A

?A

Frequencies -- 1428.8650 1430.0629 1545.1595

Red. masses -- 1.4333 1.3975 1.0996

Frc consts -- 1.7242 1.6839 1.5468

IR Inten -- 10.3527 6.1733 .4247

Raman Activ -- .0000 .0000 .0000

Depolar -- .0000 .0000 .0000

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-.04	.06	.01	.00	-.06	-.01	.02	.00	-.01
2	6	.04	-.06	-.02	-.06	.10	.02	.01	.00	.01
3	6	.02	.01	.03	-.03	-.04	.00	.01	-.03	.00
4	6	.14	.02	-.01	.03	.02	.01	.00	.00	.00
5	6	.02	.05	.00	.09	.08	.01	.01	.00	-.01
6	7	-.01	-.04	.02	-.01	-.01	.00	.00	.00	.00
7	6	.00	-.01	.00	-.01	-.01	-.01	-.07	.04	-.01
8	6	-.02	.02	-.02	.00	.00	.00	.00	.00	-.01
9	1	-.01	-.08	-.02	.08	.25	.07	-.15	.05	.00
10	1	-.18	.16	.01	.22	-.33	-.07	-.13	-.09	-.04
11	1	-.16	.18	-.02	.18	-.20	-.01	-.01	.02	-.16
12	1	-.14	.02	-.07	.30	.04	.15	.02	.26	-.15
13	1	-.60	-.14	.03	.00	.01	.02	-.01	-.02	.02
14	1	-.51	-.07	-.03	-.16	-.07	-.01	.02	-.03	-.01
15	1	-.13	-.21	-.05	-.45	-.51	-.11	-.03	-.02	-.01
16	1	.01	.03	-.05	.03	.04	-.05	.49	-.02	.32
17	1	-.15	-.17	.04	.03	-.02	-.05	-.04	-.03	.14
18	1	-.10	-.05	-.08	-.08	-.06	-.04	-.12	.19	.18
19	1	-.03	.02	.03	-.10	-.03	.08	.30	-.45	-.23
20	1	.07	-.05	.04	.00	.00	.04	.00	.00	.11
21	1	.06	-.09	-.01	-.01	-.03	.01	-.07	-.08	.04

40

41

42

?A

?A

?A

Frequencies -- 1550.8812 1552.6778 1566.3201

Red. masses -- 1.0932 1.0809 1.0930

Frc consts -- 1.5492 1.5353 1.5798

IR Inten -- 7.2193 2.7673 2.2679

Raman Activ -- .0000 .0000 .0000

Depolar -- .0000 .0000 .0000

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-.06	.01	.05	.02	-.01	-.02	-.01	.01	.00
2	6	.00	.00	.00	-.03	-.01	-.04	-.03	-.02	-.04
3	6	.00	.02	.00	-.01	.04	.00	.01	-.05	-.01
4	6	.00	.00	.00	.01	-.01	.00	.01	-.03	.01
5	6	.00	.00	.00	.00	.01	.00	.01	.00	.00
6	7	.01	.00	.00	.00	.00	.00	.00	-.01	.00
7	6	-.02	.01	.00	-.03	.02	.00	.00	.00	.00
8	6	.00	.00	-.01	.00	.01	-.01	.00	-.01	.01
9	1	.61	-.25	.01	-.16	.09	.00	.09	-.03	.00
10	1	.01	-.01	.00	.34	.27	.11	.35	.28	.11
11	1	-.02	.01	-.01	.05	-.07	.43	.04	-.08	.45
12	1	-.03	-.12	.05	-.06	-.36	.19	.06	.39	-.22
13	1	-.04	.04	-.06	-.01	.04	-.07	-.04	.12	-.21
14	1	.01	.06	.02	-.04	.07	.02	-.08	.23	.07
15	1	-.01	.00	.00	.01	-.01	-.01	-.02	-.01	.00
16	1	.18	.00	.11	.22	.00	.14	-.03	.00	-.02
17	1	.19	.10	-.61	-.06	-.03	.17	.01	-.01	-.09
18	1	.02	-.09	-.10	.16	-.28	-.27	-.18	.29	.28
19	1	.11	-.16	-.08	.14	-.19	-.10	-.03	.03	.02
20	1	.01	.00	.09	.02	-.01	.11	-.01	.00	-.09

S118

```

21 1  -.05  -.07  .03  -.07  -.09  .04  .06  .06  -.04
      43      44      45
      ?A      ?A      ?A
Frequencies -- 1576.6237      1592.8889      3023.7651
Red. masses -- 1.0925      1.1062      1.0675
Frc consts -- 1.6001      1.6536      5.7504
IR Inten -- 5.1806      4.0660      50.4776
Raman Activ -- .0000      .0000      .0000
Depolar -- .0000      .0000      .0000
Atom AN  X   Y   Z   X   Y   Z   X   Y   Z
 1 6  -.01  .01  .01  .00  .00  .00  .00  .00  .00
 2 6  -.01  -.01  -.02  -.01  -.01  -.01  .00  .00  .00
 3 6  .00  -.01  .00  .00  -.01  -.01  .00  .00  .00
 4 6  -.01  .06  -.02  -.01  .03  -.01  .00  .01  -.01
 5 6  .00  .00  .00  .00  -.01  .01  .00  .00  .00
 6 7  .00  .00  .00  -.01  .01  -.01  .00  .00  .00
 7 6  -.01  .01  .00  .02  -.01  .00  .00  .00  .00
 8 6  -.01  -.03  .03  .03  .04  -.06  .02  .00  .07
 9 1  .07  -.05  -.01  .02  -.02  .00  .00  .00  .00
10 1  .14  .15  .05  .10  .09  .03  .00  .00  .02
11 1  .01  -.03  .20  .01  -.02  .13  .00  .00  .00
12 1  .00  .03  -.02  .02  .12  -.07  -.01  .01  .02
13 1  .03  -.30  .49  .04  -.14  .25  .01  -.05  -.04
14 1  .12  -.54  -.18  .10  -.27  -.09  -.01  -.02  .10
15 1  -.01  -.01  .00  .02  .03  .02  .00  .00  -.02
16 1  .07  .00  .05  -.12  .00  -.08  -.01  .02  .02
17 1  .02  .02  -.07  .01  .02  -.02  .00  .00  .00
18 1  -.01  .02  .02  -.03  .10  .10  .00  .00  .00
19 1  .04  -.07  -.03  -.07  .10  .06  .01  .01  .01
20 1  -.06  .01  -.31  .09  .00  .57  .16  .19  .02
21 1  .17  .25  -.12  -.36  -.43  .21  -.36  -.20  -.87
      46      47      48
      ?A      ?A      ?A
Frequencies -- 3042.1393      3089.2087      3089.6107
Red. masses -- 1.0647      1.0641      1.0779
Frc consts -- 5.8052      5.9829      6.0624
IR Inten -- 53.3833      9.1207      31.1921
Raman Activ -- .0000      .0000      .0000
Depolar -- .0000      .0000      .0000
Atom AN  X   Y   Z   X   Y   Z   X   Y   Z
 1 6  .00  .00  .01  .00  .00  .00  -.02  .00  .03
 2 6  .00  .00  .00  -.02  -.01  -.05  -.01  .00  -.03
 3 6  .00  .00  .00  -.01  .04  .01  .00  -.02  .01
 4 6  .00  .05  -.05  .00  .00  .00  .00  -.01  -.01
 5 6  .00  .00  .00  .00  .00  .03  .00  .01  -.06
 6 7  .00  .00  .00  .00  .00  .00  .00  .00  .00
 7 6  .00  .00  .00  .00  .00  .00  .00  .00  .00
 8 6  .00  .00  -.01  .00  .00  .00  .00  .00  .00
 9 1  .00  .01  -.05  .00  .01  -.03  .02  .09  -.38
10 1  .00  .01  -.02  -.09  -.18  .58  -.06  -.13  .42
11 1  .00  .00  .00  .31  .26  -.02  .13  .11  -.01
12 1  .00  .00  -.01  .19  -.17  -.32  -.01  .00  .01
13 1  .06  -.30  -.23  .01  -.03  -.02  -.02  .11  .08
14 1  .00  -.24  .88  .00  .00  .00  .00  -.01  .03
15 1  .00  .00  .02  .01  .06  -.33  -.02  -.12  .69
16 1  .00  -.01  -.01  .00  .00  .00  .00  .02  .01
17 1  -.03  .02  -.01  -.05  .02  -.02  .17  -.08  .06
18 1  .00  .00  .00  -.10  -.27  .26  .06  .18  -.17
19 1  .00  .00  .00  .02  .00  .02  -.03  -.01  -.03
20 1  -.01  -.01  .00  .00  .00  .00  .00  -.01  .00
21 1  .04  .03  .11  .00  .00  .01  .00  .00  -.01
      49      50      51
      ?A      ?A      ?A
Frequencies -- 3093.1831      3099.6187      3105.2656
Red. masses -- 1.0790      1.0683      1.0859
Frc consts -- 6.0825      6.0472      6.1694
IR Inten -- 12.9607      31.2638      73.5688
Raman Activ -- .0000      .0000      .0000
Depolar -- .0000      .0000      .0000
Atom AN  X   Y   Z   X   Y   Z   X   Y   Z
 1 6  .03  .00  -.03  .00  .00  .00  .03  .00  -.03

```

S119

2	6	-.01	.00	-.01	-.01	.00	-.03	-.01	-.01	.00
3	6	.00	-.01	.01	.01	-.05	-.01	.00	.00	.00
4	6	-.01	.03	.05	.00	.00	.00	.01	-.04	-.06
5	6	.00	.00	-.03	.00	-.01	.04	.00	.00	-.01
6	7	.00	.00	.00	.00	.00	.00	.00	.00	.00
7	6	.00	.00	.00	.00	.00	.00	.00	.00	.00
8	6	.00	.00	.00	.00	.00	.00	.00	.00	.00
9	1	-.02	-.12	.51	.00	.00	.02	-.02	-.11	.45
10	1	-.02	-.04	.14	-.05	-.11	.35	-.01	-.01	.02
11	1	.11	.09	-.01	.13	.10	-.01	.10	.08	.00
12	1	-.01	.00	.01	-.28	.25	.46	.02	-.02	-.04
13	1	.08	-.48	-.32	.00	.03	.02	-.10	.56	.38
14	1	.00	.07	-.21	.00	-.01	.03	.00	-.09	.27
15	1	-.01	-.06	.35	.01	.07	-.43	.00	-.03	.16
16	1	.00	.01	.00	.01	-.03	-.02	.00	.01	.01
17	1	-.33	.15	-.11	-.06	.02	-.02	-.36	.16	-.12
18	1	.03	.09	-.08	.14	.37	-.34	.00	.01	-.01
19	1	-.02	-.01	-.02	.03	.01	.03	-.01	.00	-.01
20	1	.00	.00	.00	-.01	-.01	.00	-.01	-.01	.00
21	1	.00	.00	.01	.01	.01	.03	-.01	.00	-.02

52

?A

53

?A

54

?A

Frequencies -- 3127.4308 3138.5706 3142.2402

Red. masses -- 1.0947 1.1025 1.0622

Frc consts -- 6.3087 6.3987 6.1790

IR Inten -- 55.0980 12.2493 32.6282

Raman Activ -- .0000 .0000 .0000

Depolar -- .0000 .0000 .0000

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	.00	.00	.00	-.01	.00	.00	.00	.00	.00
2	6	.00	.00	.00	-.04	-.04	.02	.00	.00	.00
3	6	.00	.00	.00	.03	.01	-.06	.00	.00	-.01
4	6	.00	.00	.00	.00	.00	.00	.00	.00	.00
5	6	.00	.00	.00	.00	.00	-.01	.00	.00	.01
6	7	.00	.00	.00	.00	.00	.00	.00	.00	.00
7	6	-.01	.00	.00	.00	.00	.00	.06	-.04	.00
8	6	.06	.07	.01	.00	.00	.00	.01	.02	.00
9	1	.00	.00	-.01	.00	.01	-.05	.00	.00	-.01
10	1	.00	.00	.00	.03	.07	-.26	.00	.00	-.01
11	1	-.01	-.01	.00	.48	.40	-.01	.03	.02	.00
12	1	-.01	.01	.01	-.24	.23	.40	-.03	.03	.05
13	1	.00	-.01	-.01	.00	-.01	-.01	.00	-.01	-.01
14	1	.00	.00	.01	.00	.00	-.01	.00	.00	.00
15	1	.00	.00	.02	.00	-.02	.14	.00	.01	-.06
16	1	.03	-.09	-.07	.02	-.05	-.04	-.19	.57	.43
17	1	.00	.00	.00	.07	-.03	.02	.00	.00	.00
18	1	-.01	-.02	.02	-.12	-.34	.30	-.01	-.02	.02
19	1	.12	.04	.12	.01	.01	.01	-.43	-.14	-.44
20	1	-.58	-.74	.03	.01	.01	.00	-.12	-.15	.01
21	1	-.07	-.03	-.21	.00	.00	.00	-.01	.00	-.03

55

?A

56

?A

57

?A

Frequencies -- 3151.8077 3157.6293 3209.1769

Red. masses -- 1.1032 1.1053 1.1100

Frc consts -- 6.4572 6.4932 6.7355

IR Inten -- 27.2294 57.5684 21.0051

Raman Activ -- .0000 .0000 .0000

Depolar -- .0000 .0000 .0000

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-.05	.03	-.06	.02	-.02	.03	.00	.00	.00
2	6	-.02	-.02	.01	-.04	-.04	.03	.00	.00	.00
3	6	-.01	-.01	.03	-.02	-.01	.05	.00	.00	.00
4	6	.00	.00	-.01	.00	.00	.01	.00	.00	.00
5	6	.00	.00	.00	.00	.00	.01	.00	.00	.00
6	7	.00	.00	.00	.00	.00	.00	.00	.00	.00
7	6	.00	.00	.00	.00	.00	.00	-.03	-.05	-.07
8	6	.00	.00	.00	.00	.00	.00	.00	.00	.00
9	1	-.04	-.11	.48	.02	.07	-.31	.00	.00	.00
10	1	.01	.02	-.08	.05	.11	-.40	.00	.00	.01
11	1	.22	.18	.00	.40	.33	-.01	.00	.00	.00
12	1	.10	-.09	-.16	.18	-.17	-.29	-.02	.02	.03

S120

13	1	.00	.01	.01	.00	-.03	-.02	.00	.00	.00
14	1	.00	-.02	.06	.00	.02	-.05	.00	.00	.00
15	1	.00	.01	-.03	.00	.02	-.11	.00	-.01	.04
16	1	.00	.01	.01	.00	.02	.01	-.19	.50	.37
17	1	.65	-.29	.19	-.26	.11	-.08	.00	.00	.00
18	1	.07	.18	-.16	.12	.33	-.29	-.01	-.01	.01
19	1	.01	.00	.01	.02	.01	.02	.53	.15	.51
20	1	-.01	-.01	.00	-.01	-.02	.00	.03	.04	.00
21	1	.00	.00	-.01	.00	.00	-.02	.02	.01	.04

- Thermochemistry -

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Atom 1 has atomic number 6 and mass 12.00000

Atom 2 has atomic number 6 and mass 12.00000

Atom 3 has atomic number 6 and mass 12.00000

Atom 4 has atomic number 6 and mass 12.00000

Atom 5 has atomic number 6 and mass 12.00000

Atom 6 has atomic number 7 and mass 14.00307

Atom 7 has atomic number 6 and mass 12.00000

Atom 8 has atomic number 6 and mass 12.00000

Atom 9 has atomic number 1 and mass 1.00783

Atom 10 has atomic number 1 and mass 1.00783

Atom 11 has atomic number 1 and mass 1.00783

Atom 12 has atomic number 1 and mass 1.00783

Atom 13 has atomic number 1 and mass 1.00783

Atom 14 has atomic number 1 and mass 1.00783

Atom 15 has atomic number 1 and mass 1.00783

Atom 16 has atomic number 1 and mass 1.00783

Atom 17 has atomic number 1 and mass 1.00783

Atom 18 has atomic number 1 and mass 1.00783

Atom 19 has atomic number 1 and mass 1.00783

Atom 20 has atomic number 1 and mass 1.00783

Atom 21 has atomic number 1 and mass 1.00783

Molecular mass: 111.10480 amu.

Principal axes and moments of inertia in atomic units:

	1	2	3
EIGENVALUES --	526.54427	880.88326	1179.18027
X	.99993	-.01116	-.00409
Y	.01111	.99987	-.01204
Z	.00423	.01200	.99992

THIS MOLECULE IS AN ASYMMETRIC TOP.

ROTATIONAL SYMMETRY NUMBER 1.

WARNING-- ASSUMPTION OF CLASSICAL BEHAVIOR FOR ROTATION
MAY CAUSE SIGNIFICANT ERROR

ROTATIONAL TEMPERATURES (KELVIN) .16449 .09833 .07345

ROTATIONAL CONSTANTS (GHZ) 3.42752 2.04879 1.53050

1 IMAGINARY FREQUENCIES IGNORED.

Zero-point vibrational energy 519824.8 (Joules/Mol)

124.24110 (Kcal/Mol)

WARNING-- EXPLICIT CONSIDERATION OF 6 DEGREES OF FREEDOM AS
VIBRATIONS MAY CAUSE SIGNIFICANT ERRORVIBRATIONAL TEMPERATURES: 203.32 403.36 501.74 542.58 634.27
(KELVIN) 662.58 902.22 959.83 1118.59 1149.26

1248.37	1298.50	1362.84	1374.26	1415.94
1433.87	1458.02	1531.20	1566.82	1606.33
1656.25	1691.30	1705.46	1747.73	1772.71
1829.19	1845.08	1864.76	1872.14	1898.51
1925.93	1960.71	1990.47	2021.34	2042.89
2055.81	2057.53	2223.13	2231.36	2233.94
2253.57	2268.40	2291.80	4350.50	4376.93
4444.66	4445.24	4450.37	4459.63	4467.76
4499.65	4515.68	4520.96	4534.72	4543.10
4617.26				

Zero-point correction= .197991 (Hartree/Particle)

Thermal correction to Energy= .204199

Thermal correction to Enthalpy= .205143

Thermal correction to Gibbs Free Energy= .167757

Sum of electronic and zero-point Energies= -327.923079

Sum of electronic and thermal Energies= -327.916871
 Sum of electronic and thermal Enthalpies= -327.915927
 Sum of electronic and thermal Free Energies= -327.953312

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	128.137	25.454	78.685
ELECTRONIC	.000	.000	.000
TRANSLATIONAL	.889	2.981	40.032
ROTATIONAL	.889	2.981	27.794
VIBRATIONAL	126.359	19.492	10.859
VIBRATION 1	.615	1.912	2.786
VIBRATION 2	.680	1.710	1.532
VIBRATION 3	.726	1.578	1.172
VIBRATION 4	.748	1.519	1.051
VIBRATION 5	.801	1.381	.824
VIBRATION 6	.818	1.338	.765
	Q	LOG10(Q)	LN(Q)
TOTAL BOT	.688057D-77	-77.162376	-177.672936
TOTAL V=0	.806218D+14	13.906452	32.020790
VIB (BOT)	.564610D-90	-90.248251	-207.804278
VIB (BOT) 1	.143839D+01	.157876	.363523
VIB (BOT) 2	.685664D+00	-.163889	-.377368
VIB (BOT) 3	.529504D+00	-.276130	-.635814
VIB (BOT) 4	.480411D+00	-.318387	-.733112
VIB (BOT) 5	.391875D+00	-.406853	-.936813
VIB (BOT) 6	.369187D+00	-.432753	-.996452
VIB (V=0)	.661571D+01	.820576	1.889447
VIB (V=0) 1	.202281D+01	.305956	.704489
VIB (V=0) 2	.134861D+01	.129886	.299072
VIB (V=0) 3	.122827D+01	.089293	.205605
VIB (V=0) 4	.119339D+01	.076784	.176801
VIB (V=0) 5	.113527D+01	.055098	.126869
VIB (V=0) 6	.112153D+01	.049811	.114694
ELECTRONIC	.100000D+01	.000000	.000000
TRANSLATIONAL	.460320D+08	7.663060	17.644847
ROTATIONAL	.264738D+06	5.422816	12.486496

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr)		
		X	Y	Z
1	6	.000008763	.000001184	.000008064
2	6	.000001557	.000000641	-.000003934
3	6	.000018930	.000005012	-.000009797
4	6	.000003609	-.000002785	.000007335
5	6	-.000019651	-.000022203	.000025216
6	7	.000003039	.000011466	-.000014155
7	6	.000016033	.000006560	-.000021404
8	6	-.000012032	.000002500	.000015887
9	1	.000004788	-.000009827	-.000002402
10	1	-.000002952	.000011494	.000000924
11	1	-.000002494	-.000004974	.000003303
12	1	-.000000886	-.000000664	-.000003789
13	1	-.000000388	-.000001738	-.000006501
14	1	-.000004973	.000007413	.000002089
15	1	.000002794	.000003145	-.000003851
16	1	-.000010252	-.000003674	-.000000850
17	1	-.000007279	-.000000918	-.000002088
18	1	-.000000354	.000002268	.000000278
19	1	-.000008196	-.000003598	.000009066
20	1	.000002279	.000000469	.000000135
21	1	.000007666	-.000001771	-.000003525

Cartesian Forces: Max .000025216 RMS .000008586
 1\1\GINC-ARMON\Freq\RMP2-FC\6-31G(d)\C7H13N1\BELOSTOT\22-Oct-2002\0\#\n
 MP2/6-31G* OPT=(CARTESIAN, NEWTON, TS, CALCALL) GEOM=ALLCHECKPOINT GU
 ESS=CHECKPOINT\1-Azabicyclo420octane, 3-sofa transition state\0,1\C,
 -1.4811815466,-0.9625813841,-0.8597688821\C,-1.4847589285,-0.933377134
 1,0.6657344357\C,-0.0521657684,-0.9668274093,1.2280278973\C,-0.8458540
 339,0.3215428977,-1.3800476606\C,1.0003988566,-0.4102820077,0.24029453

S122

13\N,0.4970549264,0.4962261333,-0.8263204935\C,1.8122046442,0.78964080
79,0.7754284349\C,0.8196542588,1.6719784666,-0.0023190637\H,-0.9176093
221,-1.8316596627,-1.2228511734\H,-1.9900858805,-0.0124251955,0.984074
7515\H,-2.0690761588,-1.764714141,1.0752319573\H,-0.0133511575,-0.4163
841394,2.175455064\H,-0.8027952918,0.3212108991,-2.4776310293\H,-1.481
9462302,1.1710892634,-1.0826846454\H,1.5943572974,-1.2359599311,-0.172
1916348\H,1.8597348606,0.9103020635,1.8606026259\H,-2.49993474,-1.0546
831006,-1.2533816795\H,0.2219102246,-2.0008675483,1.4677080011\H,2.818
120212,0.8337434932,0.3528624298\H,1.2125742429,2.5340584935,-0.554516
2923\H,-0.0210674348,2.0121411504,0.6274669226\\Version=IBM-RS6000-G98
RevA.7\HF=-327.0456873\MP2=-328.1210695\RMSD=1.771e-09\RMSF=8.586e-06\
Dipole=-0.2447992,-0.0684577,0.342158\

Conformers of alkaloid 7aConformer 1

Item Value Threshold Converged?
 Maximum Force .000051 .000450 YES
 RMS Force .000012 .000300 YES
 Maximum Displacement .000025 .001800 YES
 RMS Displacement .000006 .001200 YES
 Predicted change in Energy=-1.558211D-06
 Optimization completed.
 -- Stationary point found.

 ! Optimized Parameters !
 ! (Angstroms and Degrees) !
 Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	.738068	.649358	-.613439
2	6	0	2.128716	.112700	-.444134
3	6	0	3.201461	.814868	.038590
4	6	0	3.063681	2.250773	.447511
5	6	0	1.771965	2.821000	-.159817
6	7	0	.634847	1.932391	.097940
7	6	0	-.348781	-.303921	-.088270
8	6	0	-1.758154	.294598	-.292648
9	6	0	-1.828408	1.713228	.334185
10	6	0	-.654175	2.563548	-.181608
11	6	0	-2.843225	-.657536	.185598
12	6	0	-3.184921	2.423153	.131010
13	6	0	-3.019868	-1.046913	1.467086
14	8	0	-2.245464	-.597627	2.476101
15	6	0	-2.546959	-1.114106	3.772659
16	6	0	-3.740582	-1.223689	-.846194
17	8	0	-4.668651	-2.089646	-.351186
18	6	0	-5.556054	-2.654375	-1.325332
19	8	0	-3.678888	-.961196	-2.035702
20	6	0	-3.639558	2.645748	-1.319665
21	7	0	2.524544	-1.171721	-.780082
22	6	0	4.333895	-.072838	.017243
23	6	0	3.872095	-1.315537	-.505948
24	6	0	5.686932	.047710	.376242
25	6	0	6.531762	-1.044256	.212476
26	6	0	6.052076	-2.263776	-.305423
27	6	0	4.717906	-2.415333	-.671299
28	1	0	.549249	.801808	-1.701406
29	1	0	3.027223	2.350501	1.541826
30	1	0	3.919704	2.847297	.103879
31	1	0	1.544867	3.793965	.289935
32	1	0	1.919210	2.990865	-1.245378
33	1	0	-.290791	-1.263855	-.618966
34	1	0	-.162479	-.496553	.972735
35	1	0	-1.906119	.399518	-1.372916
36	1	0	-1.676859	1.606471	1.414911
37	1	0	-.671081	3.536469	.325044
38	1	0	-.773499	2.764055	-1.265867
39	1	0	-3.956089	1.845792	.656869
40	1	0	-3.136896	3.394417	.644273
41	1	0	-3.804714	-1.746968	1.742831
42	1	0	-2.400378	-2.200492	3.806371
43	1	0	-1.852568	-.632089	4.461944
44	1	0	-3.576923	-.872641	4.062214
45	1	0	-6.229341	-3.304347	-.764566
46	1	0	-6.119489	-1.869980	-1.837958
47	1	0	-4.999360	-3.231061	-2.069162
48	1	0	-4.606015	3.163386	-1.336272
49	1	0	-2.931212	3.263854	-1.882789

50	1	0	-3.761812	1.700474	-1.858308
51	1	0	1.924386	-1.891004	-1.151528
52	1	0	6.068067	.983484	.777771
53	1	0	7.579710	-.959408	.487753
54	1	0	6.735008	-3.100925	-.422586
55	1	0	4.349237	-3.356393	-1.072302

 Rotational constants (GHZ): .3154319 .0967923 .0878943
 Isotopes: C-12,C-12,C-12,C-12,C-12,N-14,C-12,C-12,C-12,C-12,C-12,C-12,O-16,
 C-12,C-12,O-16,C-12,O-16,C-12,N-14,C-12,C-12,C-12,C-12,C-12,H-1,H-1,H-1,H-1,
 H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,
 H-1,H-1,H-1,H-1

Dipole moment (Debye):

X= -3.6574 Y= -1.9874 Z= 2.8405 Tot= 5.0393

Quadrupole moment (Debye-Ang):

XX= -158.3437 YY= -146.8345 ZZ= -154.5292

XY= 10.0360 XZ= -10.2661 YZ= .0275

Octapole moment (Debye-Ang**2):

XXX= -166.7915 YYY= -34.9240 ZZZ= 71.7833 XYY= -27.0499

XXY= -46.7388 XXZ= 37.2772 XZZ= -51.2050 YZZ= -22.9994

YYZ= -7.1894 XYZ= 13.9456

Hexadecapole moment (Debye-Ang**3):

XXXX= -11895.1279 YYYY= -2974.6929 ZZZZ= -1395.9385 XXXY= 399.8050

XXXZ= 134.7258 YYYY= 134.1523 YYYZ= 64.6895 ZZZX= -167.1902

ZZYZ= -56.3176 XYYX= -2362.8978 XXZZ= -2364.6801 YYZZ= -749.1634

XXYZ= 78.1891 YYXZ= -2.5847 ZZXY= 96.1813

N-N= 2.516469800693D+03 E-N= -7.800089643671D+03 KE= 1.179161329741D+03

1\1\GINC-ARMONIFOpt\RB3LYP\6-31G(d)\C22H28N2O3\BELOSTOT\29-Jul-2002\1\
 \# B3LYP/6-31G* OPT=Z-MATRIX GEOM=ALLCHECKPOINT GUESS=CHECKPOINT\Dihiy

drocorynantheine, lowest energy trans conformer\0,1\C\1,1\2\C,2,r3,1
 ,a3\C,3,r4,2,a4,1,d4,0\C,4,r5,3,a5,2,d5,0\N,1,r6,2,a6,3,d6,0\C,1,r7,2,
 a7,3,d7,0\C,7,r8,1,a8,2,d8,0\C,8,r9,7,a9,1,d9,0\C,6,r10,1,a10,2,d10,0\
 C,8,r11,7,a11,1,d11,0\C,9,r12,8,a12,7,d12,0\C,11,r13,8,a13,7,d13,0\O,1
 3,r14,11,a14,8,d14,0\C,14,r15,13,a15,11,d15,0\C,11,r16,8,a16,7,d16,0\O
 ,16,r17,11,a17,8,d17,0\C,17,r18,16,a18,11,d18,0\O,16,r19,11,a19,8,d19,
 0\C,12,r20,9,a20,8,d20,0\N,2,r21,1,a21,3,d21,0\C,3,r22,2,a22,1,d22,0\C
 ,21,r23,2,a23,1,d23,0\C,22,r24,3,a24,2,d24,0\C,24,r25,22,a25,3,d25,0\C
 ,25,r26,24,a26,22,d26,0\C,26,r27,25,a27,24,d27,0\H,1,r28,2,a28,3,d28,0
 \H,4,r29,3,a29,2,d29,0\H,4,r30,3,a30,2,d30,0\H,5,r31,4,a31,3,d31,0\H,5
 ,r32,4,a32,3,d32,0\H,7,r33,1,a33,2,d33,0\H,7,r34,1,a34,2,d34,0\H,8,r35
 ,7,a35,1,d35,0\H,9,r36,8,a36,7,d36,0\H,10,r37,6,a37,1,d37,0\H,10,r38,6
 ,a38,1,d38,0\H,12,r39,9,a39,8,d39,0\H,12,r40,9,a40,8,d40,0\H,13,r41,11
 ,a41,8,d41,0\H,15,r42,14,a42,13,d42,0\H,15,r43,14,a43,13,d43,0\H,15,r4
 4,14,a44,13,d44,0\H,18,r45,17,a45,16,d45,0\H,18,r46,17,a46,16,d46,0\H,
 18,r47,17,a47,16,d47,0\H,20,r48,12,a48,9,d48,0\H,20,r49,12,a49,9,d49,0
 \H,20,r50,12,a50,9,d50,0\H,21,r51,2,a51,1,d51,0\H,24,r52,22,a52,3,d52,
 0\H,25,r53,24,a53,22,d53,0\H,26,r54,25,a54,24,d54,0\H,27,r55,26,a55,25
 ,d55,0\2=1.50018888\3=1.36998019\4=125.61090746\5=1.49934047\6=1
 20.99731732\7=0.4361506\8=1.5370543\9=108.95060117\10=342.7775078\
 r6=1.47067622\11=108.81761082\12=347.21017707\13=1.53811129\14=113.251
 92128\15=225.79654882\16=1.54477411\17=111.06178734\18=180.23709269\19
 =1.55253563\20=109.99257393\21=306.31525145\22=1.46221905\23=110.240
 83469\24=173.05159512\25=1.52074261\26=111.51755524\27=178.3147707
 3\28=1.54447453\29=113.99400752\30=177.60630346\31=1.35093566\32=124.89468838\
 d13=64.56575149\33=1.34895166\34=122.58054261\35=361.2
 7760688\36=1.42783546\37=115.94650838\38=180.71216683\39=1.4799914
 3\40=116.92887473\41=246.47311906\42=1.36243389\43=113.75721012\44=1
 7=178.64297608\45=1.43365413\46=115.15895861\47=179.88474753\48=1.
 21968717\49=124.53531324\50=1.23997866\51=1.53645789\52=116.78770
 078\53=300.89085048\54=1.38538023\55=124.69073313\56=181.26719335\
 r22=1.43905745\57=107.1454541\58=180.65918881\59=1.38265167\60=109
 .0759508\61=179.28824582\62=1.40503418\63=134.51446312\64=179.9742
 7036\65=1.3903042\66=19.1886493\67=180.3485358\68=1.40909451\69=121.07643339\
 d26=-0.02071169\70=1.39170543\71=121.14615897\72=360.0
 6679442\73=1.11470399\74=108.42681846\75=106.75833612\76=1.0994545
 9\77=111.18465688\78=103.39274489\79=1.09849888\80=111.29281565\81=0
 222.2405933\82=1.09567858\83=109.96411677\84=168.31785675\85=1.1
 0859304\86=109.39866606\87=285.63254595\88=1.09839628\89=109.83858
 91\90=300.68333761\91=1.09432421\92=108.65338957\93=58.37449288\94

5=1.09539093\ a35=106.90747701\ d35=63.01391761\ r36=1.09650987\ a36=107.6
2090254\ d36=296.36289049\ r37=1.09706788\ a37=107.94417961\ d37=182.76671
559\ r38=1.10907931\ a38=111.08680121\ d38=299.57584468\ r39=1.09753122\ a3
9=108.19765984\ d39=63.85495165\ r40=1.09958982\ a40=107.83321168\ d40=177
.82139381\ r41=1.08724255\ a41=121.36940009\ d41=181.1973771\ r42=1.096747
95\ a42=110.97715859\ d42=62.56569087\ r43=1.09070269\ a43=106.23474916\ d4
3=181.47097693\ r44=1.09680205\ a44=111.00072404\ d44=300.4236336\ r45=1.0
9097991\ a45=105.51073678\ d45=180.61847725\ r46=1.09339871\ a46=110.79006
124\ d46=300.24212263\ r47=1.09350742\ a47=110.78256615\ d47=61.05304568\ r
48=1.09647777\ a48=110.09062915\ d48=180.51360678\ r49=1.09586421\ a49=112
.06288797\ d49=299.71961983\ r50=1.09481659\ a50=111.86868186\ d50=60.9758
3069\ r51=1.00773597\ a51=125.51872374\ d51=358.4305887\ r52=1.08727291\ a5
2=120.38253605\ d52=0.38760513\ r53=1.08681716\ a53=119.65484091\ d53=180.
00322567\ r54=1.08671155\ a54=119.49861246\ d54=180.00500928\ r55=1.087342
52\ a55=121.08056833\ d55=179.90250169\ \Version=IBM-RS6000-G98RevA.7\HF=
-1190.3717545\RMSD=9.914e-09\RMSF=8.823e-05\Dipole=-0.7298091,1.592763
4,-0.9280199\PG=C01 [X(C22H28N2O3)]\@

Conformer 2

Item Value Threshold Converged?
 Maximum Force .000051 .000450 YES
 RMS Force .000012 .000300 YES
 Maximum Displacement .000025 .001800 YES
 RMS Displacement .000006 .001200 YES
 Predicted change in Energy=-1.558211D-06
 Optimization completed.
 -- Stationary point found.

 ! Optimized Parameters !
 ! (Angstroms and Degrees) !
 Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	.738068	.649358	-.613439
2	6	0	2.128716	.112700	-.444134
3	6	0	3.201461	.814868	.038590
4	6	0	3.063681	2.250773	.447511
5	6	0	1.771965	2.821000	-.159817
6	7	0	.634847	1.932391	.097940
7	6	0	-.348781	-.303921	-.088270
8	6	0	-1.758154	.294598	-.292648
9	6	0	-1.828408	1.713228	.334185
10	6	0	-.654175	2.563548	-.181608
11	6	0	-2.843225	-.657536	.185598
12	6	0	-3.184921	2.423153	.131010
13	6	0	-3.019868	-1.046913	1.467086
14	8	0	-2.245464	-.597627	2.476101
15	6	0	-2.546959	-1.114106	3.772659
16	6	0	-3.740582	-1.223689	-.846194
17	8	0	-4.668651	-2.089646	-.351186
18	6	0	-5.556054	-2.654375	-1.325332
19	8	0	-3.678888	-.961196	-2.035702
20	6	0	-3.639558	2.645748	-1.319665
21	7	0	2.524544	-1.171721	-.780082
22	6	0	4.333895	-.072838	.017243
23	6	0	3.872095	-1.315537	-.505948
24	6	0	5.686932	.047710	.376242
25	6	0	6.531762	-1.044256	.212476
26	6	0	6.052076	-2.263776	-.305423
27	6	0	4.717906	-2.415333	-.671299
28	1	0	.549249	.801808	-1.701406
29	1	0	3.027223	2.350501	1.541826
30	1	0	3.919704	2.847297	.103879
31	1	0	1.544867	3.793965	.289935
32	1	0	1.919210	2.990865	-1.245378
33	1	0	-.290791	-1.263855	-.618966
34	1	0	-.162479	-.496553	.972735
35	1	0	-1.906119	.399518	-1.372916
36	1	0	-1.676859	1.606471	1.414911
37	1	0	-.671081	3.536469	.325044
38	1	0	-.773499	2.764055	-1.265867
39	1	0	-3.956089	1.845792	.656869
40	1	0	-3.136896	3.394417	.644273
41	1	0	-3.804714	-1.746968	1.742831
42	1	0	-2.400378	-2.200492	3.806371
43	1	0	-1.852568	-.632089	4.461944
44	1	0	-3.576923	-.872641	4.062214
45	1	0	-6.229341	-3.304347	-.764566
46	1	0	-6.119489	-1.869980	-1.837958
47	1	0	-4.999360	-3.231061	-2.069162
48	1	0	-4.606015	3.163386	-1.336272
49	1	0	-2.931212	3.263854	-1.882789
50	1	0	-3.761812	1.700474	-1.858308
51	1	0	1.924386	-1.891004	-1.151528
52	1	0	6.068067	.983484	.777771
53	1	0	7.579710	-.959408	.487753

54	1	0	6.735008	-3.100925	-.422586
55	1	0	4.349237	-3.356393	-1.072302

Rotational constants (GHz): .3154319 .0967923 .0878943

Isotopes: C-12,C-12,C-12,C-12,C-12,N-14,C-12,C-12,C-12,C-12,C-12,O-16,
C-12,C-12,O-16,C-12,O-16,C-12,N-14,C-12,C-12,C-12,C-12,C-12,H-1,H-1,H-1,H-1,
H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,
H-1,H-1,H-1,H-1

Dipole moment (Debye):
X= -3.6574 Y= -1.9874 Z= 2.8405 Tot= 5.0393

Quadrupole moment (Debye-Ang):
XX= -158.3437 YY= -146.8345 ZZ= -154.5292
XY= 10.0360 XZ= -10.2661 YZ= .0275

Octapole moment (Debye-Ang**2):
XXX= -166.7915 YYY= -34.9240 ZZZ= 71.7833 XYY= -27.0499
XXY= -46.7388 XXZ= 37.2772 XZZ= -51.2050 YZZ= -22.9994
YYZ= -7.1894 XYZ= 13.9456

Hexadecapole moment (Debye-Ang**3):
XXXX= -11895.1279 YYYY= -2974.6929 ZZZZ= -1395.9385 XXXY= 399.8050
XXXZ= 134.7258 YYYY= 134.1523 YYYZ= 64.6895 ZZZX= -167.1902
ZZZY= -56.3176 XYYX= -2362.8978 XXZZ= -2364.6801 YYZZ= -749.1634
XXYZ= 78.1891 YYXZ= -2.5847 ZZXY= 96.1813

N-N= 2.516469800693D+03 E-N=-7.800089643671D+03 KE= 1.179161329741D+03

1\1\GINC-ARMON\FOpt\RB3LYP\6-31G(d)\C22H28N2O3\BELOSTOT\29-Jul-2002\1\
\# B3LYP/6-31G* OPT=Z-MATRIX GEOM=ALLCHECKPOINT GUESS=CHECKPOINT\Dihi
drocorynantheine, lowest energy trans conformer\0,1\1C,1,r2\0,2,r3,1
,a3\0,3,r4,2,a4,1,d4,0\0,4,r5,3,a5,2,d5,0\N,1,r6,2,a6,3,d6,0\0,1,r7,2,
a7,3,d7,0\0,7,r8,1,a8,2,d8,0\0,8,r9,7,a9,1,d9,0\0,6,r10,1,a10,2,d10,0\
C,8,r11,7,a11,1,d11,0\0,9,r12,8,a12,7,d12,0\0,11,r13,8,a13,7,d13,0\0,1
3,r14,11,a14,8,d14,0\0,14,r15,13,a15,11,d15,0\0,11,r16,8,a16,7,d16,0\0
,16,r17,11,a17,8,d17,0\0,17,r18,16,a18,11,d18,0\0,16,r19,11,a19,8,d19,
0\0,12,r20,9,a20,8,d20,0\N,2,r21,1,a21,3,d21,0\0,3,r22,2,a22,1,d22,0\0
,21,r23,2,a23,1,d23,0\0,22,r24,3,a24,2,d24,0\0,24,r25,22,a25,3,d25,0\0
,25,r26,24,a26,22,d26,0\0,26,r27,25,a27,24,d27,0\H,1,r28,2,a28,3,d28,0\
\H,4,r29,3,a29,2,d29,0\H,4,r30,3,a30,2,d30,0\H,5,r31,4,a31,3,d31,0\H,5
,r32,4,a32,3,d32,0\H,7,r33,1,a33,2,d33,0\H,7,r34,1,a34,2,d34,0\H,8,r35
,7,a35,1,d35,0\H,9,r36,8,a36,7,d36,0\H,10,r37,6,a37,1,d37,0\H,10,r38,6
,a38,1,d38,0\H,12,r39,9,a39,8,d39,0\H,12,r40,9,a40,8,d40,0\H,13,r41,11
,a41,8,d41,0\H,15,r42,14,a42,13,d42,0\H,15,r43,14,a43,13,d43,0\H,15,r4
4,14,a44,13,d44,0\H,18,r45,17,a45,16,d45,0\H,18,r46,17,a46,16,d46,0\H,
18,r47,17,a47,16,d47,0\H,20,r48,12,a48,9,d48,0\H,20,r49,12,a49,9,d49,0\
\H,20,r50,12,a50,9,d50,0\H,21,r51,2,a51,1,d51,0\H,24,r52,22,a52,3,d52,
0\H,25,r53,24,a53,22,d53,0\H,26,r54,25,a54,24,d54,0\H,27,r55,26,a55,25
,d55,0\2=1.50018888\3=1.36998019\4=125.61090746\5=1.49934047\6=1
20.99731732\7=0.4361506\8=1.5370543\9=108.95060117\10=342.7775078\
r6=1.47067622\11=108.81761082\12=347.21017707\13=1.53811129\14=113.251
92128\15=225.79654882\16=1.54477411\17=111.06178734\18=180.23709269\19
=1.55253563\20=109.99257393\21=306.31525145\22=1.46221905\23=110.240
83469\24=173.05159512\25=1.52074261\26=111.51755524\27=178.3147707
3\28=1.54447453\29=113.99400752\30=177.60630346\31=1.35093566\32=124.89468838\
d13=64.56575149\33=1.34895166\34=122.58054261\35=361.2
7760688\36=1.42783546\37=115.94650838\38=180.71216683\39=1.4799914
3\40=116.92887473\41=246.47311906\42=1.36243389\43=113.75721012\44
7=178.64297608\45=1.43365413\46=115.15895861\47=179.88474753\48=1.
21968717\49=124.53531324\50=1.23997866\51=1.53645789\52=116.78770
078\53=300.89085048\54=1.38538023\55=124.69073313\56=181.26719335\
r22=1.43905745\57=107.1454541\58=180.65918881\59=1.38265167\60=109
.0759508\61=179.28824582\62=1.40503418\63=134.51446312\64=179.9742
7036\65=1.3903042\66=119.1886493\67=180.3485358\68=1.40909451\69=121.07643339\
d26=-0.02071169\70=1.39170543\71=121.14615897\72=360.0
6679442\73=1.11470399\74=108.42681846\75=106.75833612\76=1.0994545
9\77=111.18465688\78=103.39274489\79=1.09849888\80=111.29281565\81
0=222.2405933\82=1.09567858\83=109.96411677\84=168.31785675\85=1.1
0859304\86=109.39866606\87=285.63254595\88=1.09839628\89=109.83858
91\90=300.68333761\91=1.09432421\92=108.65338957\93=58.37449288\94
5=1.09539093\95=106.90747701\96=63.01391761\97=1.09650987\98=107.6
2090254\99=296.36289049\100=1.09706788\101=107.94417961\102=182.76671
559\103=1.10907931\104=111.08680121\105=299.57584468\106=1.09753122\107
9=108.19765984\108=63.85495165\109=1.09958982\110=107.83321168\111=177
.82139381\112=1.08724255\113=121.36940009\114=181.1973771\115=1.096747

95\ a42=110.97715859\ d42=62.56569087\ r43=1.09070269\ a43=106.23474916\ d4
3=181.47097693\ r44=1.09680205\ a44=111.00072404\ d44=300.4236336\ r45=1.0
9097991\ a45=105.51073678\ d45=180.61847725\ r46=1.09339871\ a46=110.79006
124\ d46=300.24212263\ r47=1.09350742\ a47=110.78256615\ d47=61.05304568\ r
48=1.09647777\ a48=110.09062915\ d48=180.51360678\ r49=1.09586421\ a49=112
.06288797\ d49=299.71961983\ r50=1.09481659\ a50=111.86868186\ d50=60.9758
3069\ r51=1.00773597\ a51=125.51872374\ d51=358.4305887\ r52=1.08727291\ a5
2=120.38253605\ d52=0.38760513\ r53=1.08681716\ a53=119.65484091\ d53=180.
00322567\ r54=1.08671155\ a54=119.49861246\ d54=180.00500928\ r55=1.087342
52\ a55=121.08056833\ d55=179.90250169\\Version=IBM-RS6000-G98RevA.7\HF=
-1190.3717545\RMSD=9.914e-09\RMSF=8.823e-05\Dipole=-0.7298091,1.592763
4,-0.9280199\PG=C01 [X(C22H28N2O3)]\@

Conformer 3

Item Value Threshold Converged?
 Maximum Force .000015 .000450 YES
 RMS Force .000003 .000300 YES
 Maximum Displacement .000778 .001800 YES
 RMS Displacement .000123 .001200 YES
 Predicted change in Energy=-1.569565D-08
 Optimization completed.
 -- Stationary point found.

 ! Optimized Parameters !
 ! (Angstroms and Degrees) !

! Name Value Derivative information (Atomic Units) !
! r2 1.4988 -DE/DX = 0. !
! r3 1.3702 -DE/DX = 0. !
! a3 125.7435 -DE/DX = 0. !
! r4 1.4999 -DE/DX = 0. !
! a4 121.2903 -DE/DX = 0. !
! d4 358.7496 -DE/DX = 0. !
! r5 1.5381 -DE/DX = 0. !
! a5 109.0741 -DE/DX = 0. !
! d5 18.5336 -DE/DX = 0. !
! r6 1.4723 -DE/DX = 0. !
! a6 108.1635 -DE/DX = 0. !
! d6 13.2826 -DE/DX = 0. !
! r7 1.551 -DE/DX = 0. !
! a7 112.2482 -DE/DX = 0. !
! d7 247.6847 -DE/DX = 0. !
! r8 1.5477 -DE/DX = 0. !
! a8 111.5879 -DE/DX = 0. !
! d8 176.3413 -DE/DX = 0. !
! r9 1.5534 -DE/DX = 0. !
! a9 110.0426 -DE/DX = 0. !
! d9 306.5098 -DE/DX = 0. !
! r10 1.4617 -DE/DX = 0. !
! a10 110.9198 -DE/DX = 0. !
! d10 181.8794 -DE/DX = 0. !
! r11 1.5209 -DE/DX = 0. !
! a11 111.2834 -DE/DX = 0. !
! d11 178.4999 -DE/DX = 0. !
! r12 1.5443 -DE/DX = 0. !
! a12 114.3284 -DE/DX = 0. !
! d12 178.8256 -DE/DX = 0. !
! r13 1.3506 -DE/DX = 0. !
! a13 124.8624 -DE/DX = 0. !
! d13 64.205 -DE/DX = 0. !
! r14 1.3504 -DE/DX = 0. !
! a14 122.589 -DE/DX = 0. !
! d14 361.4835 -DE/DX = 0. !
! r15 1.4279 -DE/DX = 0. !
! a15 115.8047 -DE/DX = 0. !
! d15 181.9188 -DE/DX = 0. !
! r16 1.4802 -DE/DX = 0. !
! a16 116.944 -DE/DX = 0. !
! d16 246.1311 -DE/DX = 0. !
! r17 1.3622 -DE/DX = 0. !
! a17 113.79 -DE/DX = 0. !
! d17 179.0806 -DE/DX = 0. !
! r18 1.4337 -DE/DX = 0. !
! a18 115.1458 -DE/DX = 0. !
! d18 179.8322 -DE/DX = 0. !
! r19 1.2197 -DE/DX = 0. !
! a19 124.5014 -DE/DX = 0. !
! d19 -0.8392 -DE/DX = 0. !
! r20 1.5364 -DE/DX = 0. !
! a20 116.5828 -DE/DX = 0. !
! d20 300.309 -DE/DX = 0. !
! r21 1.3859 -DE/DX = 0. !

!	a21	124.5062	-DE/DX = 0.	!
!	d21	178.2739	-DE/DX = 0.	!
!	r22	1.4396	-DE/DX = 0.	!
!	a22	107.0703	-DE/DX = 0.	!
!	d22	179.0839	-DE/DX = 0.	!
!	r23	1.3828	-DE/DX = 0.	!
!	a23	109.0647	-DE/DX = 0.	!
!	d23	180.8022	-DE/DX = 0.	!
!	r24	1.405	-DE/DX = 0.	!
!	a24	134.4589	-DE/DX = 0.	!
!	d24	179.991	-DE/DX = 0.	!
!	r25	1.3904	-DE/DX = 0.	!
!	a25	119.203	-DE/DX = 0.	!
!	d25	179.7941	-DE/DX = 0.	!
!	r26	1.409	-DE/DX = 0.	!
!	a26	121.0681	-DE/DX = 0.	!
!	d26	0.0367	-DE/DX = 0.	!
!	r27	1.3918	-DE/DX = 0.	!
!	a27	121.1432	-DE/DX = 0.	!
!	d27	-0.1065	-DE/DX = 0.	!
!	r28	1.1034	-DE/DX = 0.	!
!	a28	109.3901	-DE/DX = 0.	!
!	d28	128.5956	-DE/DX = 0.	!
!	r29	1.0987	-DE/DX = 0.	!
!	a29	111.3455	-DE/DX = 0.	!
!	d29	139.3076	-DE/DX = 0.	!
!	r30	1.0994	-DE/DX = 0.	!
!	a30	110.8543	-DE/DX = 0.	!
!	d30	258.0355	-DE/DX = 0.	!
!	r31	1.1058	-DE/DX = 0.	!
!	a31	108.9154	-DE/DX = 0.	!
!	d31	76.2466	-DE/DX = 0.	!
!	r32	1.0959	-DE/DX = 0.	!
!	a32	109.9387	-DE/DX = 0.	!
!	d32	192.9977	-DE/DX = 0.	!
!	r33	1.0984	-DE/DX = 0.	!
!	a33	109.53	-DE/DX = 0.	!
!	d33	297.6509	-DE/DX = 0.	!
!	r34	1.0949	-DE/DX = 0.	!
!	a34	109.2987	-DE/DX = 0.	!
!	d34	54.3077	-DE/DX = 0.	!
!	r35	1.0961	-DE/DX = 0.	!
!	a35	107.0891	-DE/DX = 0.	!
!	d35	63.289	-DE/DX = 0.	!
!	r36	1.0978	-DE/DX = 0.	!
!	a36	107.6626	-DE/DX = 0.	!
!	d36	297.1742	-DE/DX = 0.	!
!	r37	1.0975	-DE/DX = 0.	!
!	a37	108.0734	-DE/DX = 0.	!
!	d37	179.5663	-DE/DX = 0.	!
!	r38	1.0996	-DE/DX = 0.	!
!	a38	107.1555	-DE/DX = 0.	!
!	d38	294.2434	-DE/DX = 0.	!
!	r39	1.0977	-DE/DX = 0.	!
!	a39	108.4973	-DE/DX = 0.	!
!	d39	63.3821	-DE/DX = 0.	!
!	r40	1.0998	-DE/DX = 0.	!
!	a40	107.7649	-DE/DX = 0.	!
!	d40	177.4759	-DE/DX = 0.	!
!	r41	1.0872	-DE/DX = 0.	!
!	a41	121.4238	-DE/DX = 0.	!
!	d41	181.3403	-DE/DX = 0.	!
!	r42	1.0908	-DE/DX = 0.	!
!	a42	106.2811	-DE/DX = 0.	!
!	d42	181.124	-DE/DX = 0.	!
!	r43	1.0968	-DE/DX = 0.	!
!	a43	110.9972	-DE/DX = 0.	!
!	d43	300.0903	-DE/DX = 0.	!
!	r44	1.0967	-DE/DX = 0.	!
!	a44	110.964	-DE/DX = 0.	!
!	d44	62.228	-DE/DX = 0.	!

!	r45	1.091	-DE/DX = 0.	!
!	a45	105.5115	-DE/DX = 0.	!
!	d45	180.2964	-DE/DX = 0.	!
!	r46	1.0934	-DE/DX = 0.	!
!	a46	110.7504	-DE/DX = 0.	!
!	d46	299.8977	-DE/DX = 0.	!
!	r47	1.0935	-DE/DX = 0.	!
!	a47	110.7957	-DE/DX = 0.	!
!	d47	60.7017	-DE/DX = 0.	!
!	r48	1.0964	-DE/DX = 0.	!
!	a48	110.1011	-DE/DX = 0.	!
!	d48	180.3308	-DE/DX = 0.	!
!	r49	1.0959	-DE/DX = 0.	!
!	a49	112.1286	-DE/DX = 0.	!
!	d49	299.4996	-DE/DX = 0.	!
!	r50	1.0947	-DE/DX = 0.	!
!	a50	111.8227	-DE/DX = 0.	!
!	d50	60.8122	-DE/DX = 0.	!
!	r51	1.0081	-DE/DX = 0.	!
!	a51	125.4712	-DE/DX = 0.	!
!	d51	3.7784	-DE/DX = 0.	!
!	r52	1.0873	-DE/DX = 0.	!
!	a52	120.3816	-DE/DX = 0.	!
!	d52	-0.315	-DE/DX = 0.	!
!	r53	1.0868	-DE/DX = 0.	!
!	a53	119.6574	-DE/DX = 0.	!
!	d53	179.9293	-DE/DX = 0.	!
!	r54	1.0867	-DE/DX = 0.	!
!	a54	119.5026	-DE/DX = 0.	!
!	d54	179.9015	-DE/DX = 0.	!
!	r55	1.0873	-DE/DX = 0.	!
!	a55	121.0713	-DE/DX = 0.	!
!	d55	180.028	-DE/DX = 0.	!

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

1\1\GINC-ARMON\FOpt\RB3LYP\6-31G(d)\C22H28N2O3\BELOSTOT\05-Aug-2002\1\

\# B3LYP/6-31G* OPT=Z-MATRIX GEOM=ALLCHECKPOINT GUESS=CHECKPOINT\DiHy

drocorynantheine, lowest energy cis conformer\0,1\C\C,1,r2\C,2,r3,1,a

3\C,3,r4,2,a4,1,d4,0\C,4,r5,3,a5,2,d5,0\N,1,r6,2,a6,3,d6,0\C,1,r7,2,a7

,3,d7,0\C,7,r8,1,a8,2,d8,0\C,8,r9,7,a9,1,d9,0\C,6,r10,1,a10,2,d10,0\C,

8,r11,7,a11,1,d11,0\C,9,r12,8,a12,7,d12,0\C,11,r13,8,a13,7,d13,0\O,13,

r14,11,a14,8,d14,0\C,14,r15,13,a15,11,d15,0\C,11,r16,8,a16,7,d16,0\O,1

6,r17,11,a17,8,d17,0\C,17,r18,16,a18,11,d18,0\O,16,r19,11,a19,8,d19,0\

C,12,r20,9,a20,8,d20,0\N,2,r21,1,a21,3,d21,0\C,3,r22,2,a22,1,d22,0\C,2

1,r23,2,a23,1,d23,0\C,22,r24,3,a24,2,d24,0\C,24,r25,22,a25,3,d25,0\C,2

5,r26,24,a26,22,d26,0\C,26,r27,25,a27,24,d27,0\H,1,r28,2,a28,3,d28,0\H

,4,r29,3,a29,2,d29,0\H,4,r30,3,a30,2,d30,0\H,5,r31,4,a31,3,d31,0\H,5,r

32,4,a32,3,d32,0\H,7,r33,1,a33,2,d33,0\H,7,r34,1,a34,2,d34,0\H,8,r35,7

,a35,1,d35,0\H,9,r36,8,a36,7,d36,0\H,10,r37,6,a37,1,d37,0\H,10,r38,6,a

38,1,d38,0\H,12,r39,9,a39,8,d39,0\H,12,r40,9,a40,8,d40,0\H,13,r41,11,a

41,8,d41,0\H,15,r42,14,a42,13,d42,0\H,15,r43,14,a43,13,d43,0\H,15,r44,

14,a44,13,d44,0\H,18,r45,17,a45,16,d45,0\H,18,r46,17,a46,16,d46,0\H,18

,r47,17,a47,16,d47,0\H,20,r48,12,a48,9,d48,0\H,20,r49,12,a49,9,d49,0\H

,20,r50,12,a50,9,d50,0\H,21,r51,2,a51,1,d51,0\H,24,r52,22,a52,3,d52,0\

H,25,r53,24,a53,22,d53,0\H,26,r54,25,a54,24,d54,0\H,27,r55,26,a55,25,d

55,0\|r2=1.49878709\r3=1.37016694\|a3=125.74353374\r4=1.49988545\|a4=121

.29027685\d4=358.7495687\r5=1.53811625\|a5=109.07410725\d5=18.53356788\

r6=1.4722691\|a6=108.16347628\d6=13.28260643\r7=1.55097887\|a7=112.24816

856\d7=247.68471042\r8=1.54767538\|a8=111.58789306\d8=176.34132434\r9=1

.5534201\|a9=110.042582\d9=306.50984758\r10=1.46165164\|a10=110.91984232

\d10=181.87935427\r11=1.52085939\|a11=111.28338379\d11=178.49992791\r12

=1.54432519\|a12=114.32835813\d12=178.82562454\r13=1.35057613\|a13=124.8

6237594\d13=64.20498979\r14=1.35037759\|a14=122.5890414\d14=361.4834716

7\r15=1.42791888\|a15=115.80468241\d15=181.91876245\r16=1.48016992\|a16=

116.94404102\d16=246.13108931\r17=1.36221311\|a17=113.79000842\d17=179.

08057251\r18=1.43372164\|a18=115.14579099\d18=179.8322044\r19=1.2196727

5\|a19=124.50143106\d19=-0.83919743\r20=1.53641837\|a20=116.58276572\d20

=300.30899184\r21=1.38588388\|a21=124.50621388\d21=178.27388827\r22=1.4

3956036\|a22=107.07032734\d22=179.08386915\r23=1.38278461\|a23=109.06471

892\d23=180.8021911\r24=1.4049956\|a24=134.45889929\d24=179.99100978\r2

5=1.39038558\ a25=119.20296521\ d25=179.79407177\ r26=1.40899044\ a26=121.
 06811412\ d26=0.03672659\ r27=1.39179159\ a27=121.14322681\ d27=-0.1065351
 7\ r28=1.10336211\ a28=109.39006046\ d28=128.5956115\ r29=1.09870363\ a29=1
 11.34552444\ d29=139.30760835\ r30=1.09942321\ a30=110.85427868\ d30=258.0
 3545732\ r31=1.10580674\ a31=108.91541015\ d31=76.24657757\ r32=1.09592679
 \ a32=109.93868052\ d32=192.99774614\ r33=1.09843012\ a33=109.53004398\ d33
 =297.65091208\ r34=1.09487665\ a34=109.29867316\ d34=54.30774114\ r35=1.09
 614126\ a35=107.08911305\ d35=63.28904645\ r36=1.09781827\ a36=107.6626049
 2\ d36=297.17422847\ r37=1.09748833\ a37=108.07339425\ d37=179.56632861\ r3
 8=1.09958807\ a38=107.15546129\ d38=294.24340574\ r39=1.09767819\ a39=108.
 4973365\ d39=63.38210845\ r40=1.09976217\ a40=107.76485435\ d40=177.475889
 69\ r41=1.08719219\ a41=121.42379953\ d41=181.34027609\ r42=1.09077762\ a42
 =106.28107652\ d42=181.12402295\ r43=1.09682885\ a43=110.9972412\ d43=300.
 09025614\ r44=1.09666122\ a44=110.96395018\ d44=62.22798313\ r45=1.0909683
 \ a45=105.511452\ d45=180.29644967\ r46=1.09340869\ a46=110.75044866\ d46=2
 99.89774904\ r47=1.0934772\ a47=110.79567956\ d47=60.70169698\ r48=1.09639
 465\ a48=110.10113579\ d48=180.33080196\ r49=1.0958903\ a49=112.12864091\ d
 49=299.49961456\ r50=1.09470139\ a50=111.82268775\ d50=60.81219494\ r51=1.
 0081141\ a51=125.47124972\ d51=3.77835033\ r52=1.08730479\ a52=120.3816255
 8\ d52=-0.31504488\ r53=1.08682774\ a53=119.65740893\ d53=179.92927289\ r54
 =1.08672274\ a54=119.50260132\ d54=179.90153766\ r55=1.08734516\ a55=121.0
 7128745\ d55=180.02799879\ \Version=IBM-RS6000-G98RevA.7\HF=-1190.367956
 3\ RMSD=5.690e-09\ RMSF=5.933e-05\ Dipole=-0.1526454,1.9325908,-0.8341209
 \ PG=C01 [X(C22H28N2O3)]\ \@

Conformer 4

Item Value Threshold Converged?
 Maximum Force .000351 .000450 YES
 RMS Force .000076 .000300 YES
 Maximum Displacement .000176 .001800 YES
 RMS Displacement .000038 .001200 YES
 Predicted change in Energy=-4.094750D-06
 Optimization completed.
 -- Stationary point found.

 ! Optimized Parameters !
 ! (Angstroms and Degrees) !

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	.735372	.515362	-.781983
2	6	0	2.128249	.035221	-.494104
3	6	0	3.175634	.817551	-.084293
4	6	0	3.004752	2.292759	.119210
5	6	0	1.719779	2.747717	-.590380
6	7	0	.592796	1.876012	-.245218
7	6	0	-.352855	-.382407	-.170154
8	6	0	-1.766265	.167888	-.463168
9	6	0	-1.875845	1.651339	-.020652
10	6	0	-.699761	2.445615	-.614629
11	6	0	-2.841593	-.740609	.111829
12	6	0	-3.229476	2.270564	-.419504
13	6	0	-3.029124	-.979083	1.427950
14	8	0	-2.277133	-.398399	2.386614
15	6	0	-2.583073	-.772271	3.729946
16	6	0	-3.711961	-1.442429	-.858832
17	8	0	-4.649901	-2.241383	-.275940
18	6	0	-5.505702	-2.939255	-1.189872
19	8	0	-3.618630	-1.338888	-2.069431
20	6	0	-3.488510	3.670653	.151573
21	7	0	2.553390	-1.276001	-.635409
22	6	0	4.320314	-.043423	.053029
23	6	0	3.893361	-1.355333	-.304421
24	6	0	5.659214	.151386	.432114
25	6	0	6.524314	-.936805	.448563
26	6	0	6.079091	-2.225426	.092421
27	6	0	4.759730	-2.451522	-.288426
28	1	0	.582189	.522804	-1.885764
29	1	0	2.939107	2.541322	1.188224
30	1	0	3.859270	2.853266	-.283724
31	1	0	1.462588	3.766632	-.280625
32	1	0	1.893432	2.774801	-1.684904
33	1	0	-.275008	-1.396138	-.585828
34	1	0	-.184833	-.450188	.908996
35	1	0	-1.906960	.144436	-1.550846
36	1	0	-1.777466	1.692341	1.071484
37	1	0	-.725494	3.474152	-.239576
38	1	0	-.821736	2.503859	-1.718342
39	1	0	-3.303989	2.300753	-1.516232
40	1	0	-4.030736	1.602234	-.081284
41	1	0	-3.804873	-1.657042	1.775301
42	1	0	-3.615045	-.504030	3.987317
43	1	0	-2.434191	-1.848212	3.881873
44	1	0	-1.893047	-.216537	4.366107
45	1	0	-6.184077	-3.523516	-.566410
46	1	0	-6.066787	-2.235136	-1.810357
47	1	0	-4.923714	-3.596185	-1.842184
48	1	0	-4.493562	4.018458	-.113698
49	1	0	-3.415368	3.671167	1.246449
50	1	0	-2.778220	4.413815	-.227525
51	1	0	1.976047	-2.050919	-.921270

52	1	0	6.013902	1.140958	.709716
53	1	0	7.561492	-.794919	.740615
54	1	0	6.777431	-3.057768	.114160
55	1	0	4.417787	-3.446076	-.564526

Rotational constants (GHZ): .3011724 .0980240 .0865943
 Isotopes: C-12,C-12,C-12,C-12,C-12,N-14,C-12,C-12,C-12,C-12,C-12,C-12,C-12,O-16,
 C-12,C-12,O-16,C-12,O-16,C-12,N-14,C-12,C-12,C-12,C-12,C-12,H-1,H-1,H-1,H-1,
 H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,
 H-1,H-1,H-1,H-1

Dipole moment (Debye):

X= -3.6431 Y= -1.5836 Z= 2.9318 Tot= 4.9372

Quadrupole moment (Debye-Ang):

XX= -158.3011 YY= -146.5309 ZZ= -155.4056

XY= 8.1869 XZ= -10.8025 YZ= -1.6760

Octapole moment (Debye-Ang**2):

XXX= -166.5746 YYY= -43.9872 ZZZ= 70.8621 XYY= -24.3411

XXY= -42.3173 XXZ= 38.5665 XZZ= -51.9911 YZZ= -11.6415

YYZ= -9.4165 XYZ= 12.3025

Hexadecapole moment (Debye-Ang**3):

XXXX= -11853.9280 YYYY= -3275.5704 ZZZZ= -1302.5676 XXXY= 408.0078

XXXZ= 124.2096 YYYY= 157.6437 YYYZ= 51.2598 ZZZX= -183.4705

ZZZY= -39.5238 XXYY= -2378.1892 XXZZ= -2343.2596 YYZZ= -807.0147

XXYZ= 42.2497 YXZ= 16.5522 ZZX= 72.7877

N-N= 2.506461911356D+03 E-N= -7.780037295667D+03 KE= 1.179167343145D+03

1\1\GINC-ESHEL\FOpt\RB3LYP\6-31G(d)\C22H28N2O3\BELOSTOT\07-Aug-2002\1\
 \# B3LYP/6-31G* OPT=Z-MATRIX GEOM=ALLCHECKPOINT GUESS=CHECKPOINT\DiHy

drocorynantheine, low energy trans conformer, min 2\0,1\C\1,r2\C,2,
 r3,1,a3\C,3,r4,2,a4,1,d4,0\C,4,r5,3,a5,2,d5,0\N,1,r6,2,a6,3,d6,0\C,1,r
 7,2,a7,3,d7,0\C,7,r8,1,a8,2,d8,0\C,8,r9,7,a9,1,d9,0\C,6,r10,1,a10,2,d1
 0,0\C,8,r11,7,a11,1,d11,0\C,9,r12,8,a12,7,d12,0\C,11,r13,8,a13,7,d13,0
 \O,13,r14,11,a14,8,d14,0\C,14,r15,13,a15,11,d15,0\C,11,r16,8,a16,7,d16
 ,0\O,16,r17,11,a17,8,d17,0\C,17,r18,16,a18,11,d18,0\O,16,r19,11,a19,8,
 d19,0\C,12,r20,9,a20,8,d20,0\N,2,r21,1,a21,3,d21,0\C,3,r22,2,a22,1,d22
 ,0\C,21,r23,2,a23,1,d23,0\C,22,r24,3,a24,2,d24,0\C,24,r25,22,a25,3,d25
 ,0\C,25,r26,24,a26,22,d26,0\C,26,r27,25,a27,24,d27,0\H,1,r28,2,a28,3,d
 28,0\H,4,r29,3,a29,2,d29,0\H,4,r30,3,a30,2,d30,0\H,5,r31,4,a31,3,d31,0
 \H,5,r32,4,a32,3,d32,0\H,7,r33,1,a33,2,d33,0\H,7,r34,1,a34,2,d34,0\H,8
 ,r35,7,a35,1,d35,0\H,9,r36,8,a36,7,d36,0\H,10,r37,6,a37,1,d37,0\H,10,r
 38,6,a38,1,d38,0\H,12,r39,9,a39,8,d39,0\H,12,r40,9,a40,8,d40,0\H,13,r4
 1,11,a41,8,d41,0\H,15,r42,14,a42,13,d42,0\H,15,r43,14,a43,13,d43,0\H,1
 5,r44,14,a44,13,d44,0\H,18,r45,17,a45,16,d45,0\H,18,r46,17,a46,16,d46,
 0\H,18,r47,17,a47,16,d47,0\H,20,r48,12,a48,9,d48,0\H,20,r49,12,a49,9,d
 49,0\H,20,r50,12,a50,9,d50,0\H,21,r51,2,a51,1,d51,0\H,24,r52,22,a52,3,
 d52,0\H,25,r53,24,a53,22,d53,0\H,26,r54,25,a54,24,d54,0\H,27,r55,26,a5
 5,25,d55,0\r2=1.50117186\r3=1.37003697\r4=1.25.73707844\r5=1.49895057\
 a4=121.02689169\d4=-0.02843292\r5=1.53676949\r6=108.90462359\d5=343.00
 497585\r6=1.46963072\r7=108.42727015\d6=346.36786231\r7=1.5377129\r8=1
 13.17879909\d7=225.230535\r8=1.54480089\r9=111.34942972\d8=178.6500078
 4\r9=1.55191996\r10=110.55012109\d9=306.802588\r10=1.46000511\r10=110.7
 7399272\d10=174.28238452\r11=1.52063138\r11=111.25158051\d11=178.52808
 504\r12=1.54105091\r12=111.85840628\d12=174.61361432\r13=1.35063368\r1
 3=124.89981765\d13=64.58329856\r14=1.34971131\r14=122.60211904\d14=1.3
 6654707\r15=1.42755808\r15=115.86737491\d15=181.12897317\r16=1.4806332
 \a16=116.8072796\d16=246.6370743\r17=1.36301911\r17=113.70315797\d17=1
 79.8366191\r18=1.43342019\r18=115.05929318\d18=180.22809221\r19=1.2185
 9868\r19=124.46982919\d19=0.10518688\r20=1.53410463\r20=114.75169307\d
 20=171.96221826\r21=1.38564581\r21=124.59645775\d21=181.5447992\r22=1.
 43889648\r22=107.16013564\d22=180.81089243\r23=1.38252285\r23=109.1025
 9587\d23=179.11761018\r24=1.40510114\r24=134.49393862\d24=180.05178526
 \r25=1.39026201\r25=119.18371684\d25=180.35156002\r26=1.40911555\r26=1
 21.07734541\d26=-0.01099685\r27=1.391718\r27=121.14874244\d27=360.0512
 7285\r28=1.11438459\r28=108.64015305\d28=105.91242086\r29=1.09949235\r
 29=111.17988477\d29=103.61226395\r30=1.09851079\r30=111.32651236\d30=2
 22.46282034\r31=1.09557446\r31=109.94235804\r31=168.01313549\r32=1.108
 54479\r32=109.39943249\r32=285.30054486\r33=1.09840651\r33=109.7610094
 4\r33=299.15311457\r34=1.09425317\r34=108.65622122\d34=56.76847708\r35
 =1.09698978\r35=107.32546929\d35=63.28736316\r36=1.09732429\r36=108.25
 095137\d36=294.40537709\r37=1.09508642\r37=107.49219158\d37=183.223263

93\r38=1.11195985\ a38=111.63501132\ d38=299.9696961\ r39=1.0996704\ a39=1
 09.18839216\ d39=295.38134555\ r40=1.09684758\ a40=108.48301848\ d40=50.41
 008332\ r41=1.08722905\ a41=121.36490771\ d41=181.29367514\ r42=1.09688711
 \ a42=111.00039756\ d42=299.10960556\ r43=1.09676609\ a43=110.98857139\ d43
 =61.23217708\ r44=1.09072275\ a44=106.2493139\ d44=180.14664807\ r45=1.090
 99037\ a45=105.52171593\ d45=179.91380432\ r46=1.09343509\ a46=110.7724353
 9\ d46=299.51317394\ r47=1.09351664\ a47=110.79747043\ d47=60.29882835\ r48
 =1.0961138\ a48=110.75189871\ d48=183.95206706\ r49=1.09731652\ a49=111.13
 697388\ d49=303.50590593\ r50=1.09568125\ a50=112.38057579\ d50=64.1032041
 2\ r51=1.00774017\ a51=125.5077851\ d51=358.33852193\ r52=1.08725278\ a52=1
 20.39288743\ d52=0.38961225\ r53=1.08681397\ a53=119.65862483\ d53=180.005
 32852\ r54=1.08671258\ a54=119.49418675\ d54=179.98805167\ r55=1.08733281\
 a55=121.07843606\ d55=179.90256473\\Version=IBM-RS6000-G98RevA.7\HF=-11
90.3724815\RMSD=7.045e-09\RMSF=8.176e-05\Dipole=-0.7087674,1.5631812,-
 0.9094481\PG=C01 [X(C22H28N2O3)]\@

Conformer 5

Maximum Force .000097 .000450 YES
 RMS Force .000024 .000300 YES
 Maximum Displacement .001686 .001800 YES
 RMS Displacement .000387 .001200 YES
 Predicted change in Energy=-2.038221D-07
 Optimization completed.
 -- Stationary point found.

 ! Optimized Parameters !
 ! (Angstroms and Degrees) !

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-.747821	.612743	.664096
2	6	0	-2.142725	.116827	.415023
3	6	0	-3.174933	.857848	-.096360
4	6	0	-2.980224	2.294190	-.478092
5	6	0	-1.693107	2.815893	.179686
6	7	0	-.576708	1.891671	-.038707
7	6	0	.341429	-.368858	.201570
8	6	0	1.750890	.202203	.472991
9	6	0	1.894147	1.603739	-.179918
10	6	0	.718873	2.488339	.270892
11	6	0	2.837598	-.787887	.087075
12	6	0	3.247897	2.260389	.151509
13	6	0	3.647944	-1.359199	1.004637
14	8	0	3.556040	-1.080258	2.322302
15	6	0	4.516911	-1.720480	3.160584
16	6	0	3.000227	-1.171054	-1.331657
17	8	0	4.005705	-2.069484	-1.539546
18	6	0	4.192928	-2.466836	-2.904302
19	8	0	2.321906	-.746194	-2.250721
20	6	0	3.522244	3.572877	-.593953
21	7	0	-2.588733	-1.161011	.713199
22	6	0	-4.330018	.000919	-.143653
23	6	0	-3.924167	-1.264817	.370088
24	6	0	-5.662026	.165766	-.559037
25	6	0	-6.540435	-.907446	-.461266
26	6	0	-6.115275	-2.151356	.046098
27	6	0	-4.803644	-2.346023	.468718
28	1	0	-.618120	.761911	1.761851
29	1	0	-2.903748	2.405954	-1.569041
30	1	0	-3.828517	2.913033	-.155117
31	1	0	-1.417771	3.782940	-.255410
32	1	0	-1.874352	2.985850	1.260389
33	1	0	.234276	-1.321140	.739241
34	1	0	.214602	-.566585	-.866256
35	1	0	1.837930	.346285	1.558255
36	1	0	1.816782	1.477997	-1.265840
37	1	0	.767907	3.452537	-.245709
38	1	0	.821270	2.702201	1.358136
39	1	0	3.312928	2.432496	1.236413
40	1	0	4.047582	1.548908	-.088242
41	1	0	4.411359	-2.078869	.720001
42	1	0	4.449722	-2.812201	3.075828
43	1	0	5.534741	-1.395622	2.912483
44	1	0	4.279707	-1.420852	4.182467
45	1	0	5.022282	-3.175548	-2.890753
46	1	0	3.289943	-2.941643	-3.297877
47	1	0	4.436978	-1.603801	-3.529778
48	1	0	4.534754	3.935897	-.382581
49	1	0	3.438106	3.434062	-1.678784
50	1	0	2.825977	4.368416	-.306405
51	1	0	-2.012621	-1.918029	1.045469
52	1	0	-6.000638	1.120291	-.954466

53	1	0	-7.572143	-.788851	-.781727
54	1	0	-6.823150	-2.973454	.109825
55	1	0	-4.477177	-3.305973	.861522

Rotational constants (GHZ): .2916947 .0974315 .0879899
 Isotopes: C-12,C-12,C-12,C-12,C-12,N-14,C-12,C-12,C-12,C-12,C-12,C-12,O-16,
 C-12,C-12,O-16,C-12,O-16,C-12,N-14,C-12,C-12,C-12,C-12,C-12,C-12,H-1,H-1,H-1,H-1,
 H-1,
 H-1,H-1,H-1,H-1

Dipole moment (Debye):

X= 5.3781 Y= -2.3743 Z= 2.9865 Tot= 6.5940

Quadrupole moment (Debye-Ang):

XX= -149.0795 YY= -145.6000 ZZ= -155.5481

XY= -11.9121 XZ= 7.0869 YZ= -4.4865

Octapole moment (Debye-Ang**2):

XXX= 198.4570 YYY= -39.2031 ZZZ= 15.8954 XYY= 25.8896

XXY= -53.6839 XXZ= 9.3729 XZZ= 82.0706 YZZ= -33.8745

YYZ= 1.1382 XYZ= 5.4994

Hexadecapole moment (Debye-Ang**3):

XXXX= -11771.4786 YYYY= -3227.8888 ZZZZ= -1548.1744 XXXY= -355.1426

XXXZ= 248.7574 YYYY= -126.1171 YYYZ= -7.4930 ZZZX= 55.5122

ZZZY= -2.3940 XYYZ= -2398.8838 XXZZ= -2139.8545 YYZZ= -768.4333

XXYZ= -65.9880 YYXZ= -32.6305 ZZXY= -177.5452

N-N= 2.504452740335D+03 E-N= -7.776211628557D+03 KE= 1.179168158494D+03
 1\1\GINC-ARMON\FOpt\RB3LYP/6-31G(d)\C22H28N2O3\BELOSTOT\26-Aug-2002\1\
 \# B3LYP/6-31G* OPT=Z-MATRIX GEOM=ALLCHECKPOINT GUESS=CHECKPOINT\DiHy
 drocorynantheine, low energy trans conformer, min 4\0,1\C\1,r2\C,2,
 r3,1,a3\C,3,r4,2,a4,1,d4,0\C,4,r5,3,a5,2,d5,0\N,1,r6,2,a6,3,d6,0\C,1,r
 7,2,a7,3,d7,0\C,7,r8,1,a8,2,d8,0\C,8,r9,7,a9,1,d9,0\C,6,r10,1,a10,2,d1
 0,0\C,8,r11,7,a11,1,d11,0\C,9,r12,8,a12,7,d12,0\C,11,r13,8,a13,7,d13,0
 \O,13,r14,11,a14,8,d14,0\C,14,r15,13,a15,11,d15,0\C,11,r16,8,a16,7,d16
 ,0\O,16,r17,11,a17,8,d17,0\C,17,r18,16,a18,11,d18,0\O,16,r19,11,a19,8,
 d19,0\C,12,r20,9,a20,8,d20,0\N,2,r21,1,a21,3,d21,0\C,3,r22,2,a22,1,d22
 ,0\C,21,r23,2,a23,1,d23,0\C,22,r24,3,a24,2,d24,0\C,24,r25,22,a25,3,d25
 ,0\C,25,r26,24,a26,22,d26,0\C,26,r27,25,a27,24,d27,0\H,1,r28,2,a28,3,d
 28,0\H,4,r29,3,a29,2,d29,0\H,4,r30,3,a30,2,d30,0\H,5,r31,4,a31,3,d31,0
 \H,5,r32,4,a32,3,d32,0\H,7,r33,1,a33,2,d33,0\H,7,r34,1,a34,2,d34,0\H,8
 ,r35,7,a35,1,d35,0\H,9,r36,8,a36,7,d36,0\H,10,r37,6,a37,1,d37,0\H,10,r
 38,6,a38,1,d38,0\H,12,r39,9,a39,8,d39,0\H,12,r40,9,a40,8,d40,0\H,13,r4
 1,11,a41,8,d41,0\H,15,r42,14,a42,13,d42,0\H,15,r43,14,a43,13,d43,0\H,1
 5,r44,14,a44,13,d44,0\H,18,r45,17,a45,16,d45,0\H,18,r46,17,a46,16,d46
 ,0\H,18,r47,17,a47,16,d47,0\H,20,r48,12,a48,9,d48,0\H,20,r49,12,a49,9,d
 49,0\H,20,r50,12,a50,9,d50,0\H,21,r51,2,a51,1,d51,0\H,24,r52,22,a52,3,
 d52,0\H,25,r53,24,a53,22,d53,0\H,26,r54,25,a54,24,d54,0\H,27,r55,26,a5
 5,25,d55,0\H,2=1.50124236\H,3=1.36969934\H,4=125.69353965\H,5=1.49890311\
 a4=121.03886218\H,6=0.53396494\H,7=1.53672275\H,8=108.97235552\H,9=343.025
 71404\H,10=1.46930813\H,11=108.44443877\H,12=345.62981066\H,13=1.53751006\H,14=1
 13.41939801\H,15=224.11138743\H,16=1.54478562\H,17=110.9481693\H,18=179.504647
 04\H,19=1.55277693\H,20=110.11842758\H,21=305.35119425\H,22=1.45958721\H,23=11
 0.96135116\H,24=174.52406926\H,25=1.51991504\H,26=111.52629278\H,27=177.04
 464991\H,28=1.5406731\H,29=112.04341529\H,30=175.76221869\H,31=1.35091721\
 a13=122.13456451\H,32=246.41884656\H,33=1.34999826\H,34=122.32541545\H,35=359.3499337\
 r15=1.42684076\H,36=115.77773378\H,37=182.49534875\H,38=1.478
 5352\H,39=119.41251098\H,40=64.86202072\H,41=1.36432416\H,42=113.44890239\
 d17=180.28037032\H,43=1.43370117\H,44=115.07446412\H,45=179.92195044\H,46=1
 2.1873062\H,47=124.8933562\H,48=360.30897883\H,49=1.53414612\H,50=114.659
 93555\H,51=173.18380356\H,52=1.38589423\H,53=124.60454891\H,54=182.2044806
 4\H,55=1.43902156\H,56=107.15807378\H,57=181.0498362\H,58=1.38270965\H,59=1
 09.06547298\H,60=179.17801582\H,61=1.40497868\H,62=134.49489248\H,63=180.0
 9848865\H,64=1.39030419\H,65=119.18527898\H,66=180.07896551\H,67=1.4090743
 6\H,68=121.07295725\H,69=360.00580783\H,70=1.3917181\H,71=121.14385752\H,72=360.14585014\
 r28=1.11541004\H,73=108.39141208\H,74=104.93668429\H,75=1.0
 9932277\H,76=111.05068871\H,77=103.5890902\H,78=1.09858114\H,79=111.384318
 58\H,80=222.4283084\H,81=1.09558095\H,82=109.88695404\H,83=167.75006372\H,84=2
 1.10889748\H,85=109.40791918\H,86=284.98284835\H,87=1.09882285\H,88=109.
 6946734\H,89=299.82280994\H,90=1.09335787\H,91=109.09176042\H,92=57.996839
 55\H,93=1.09824089\H,94=107.12364111\H,95=61.1864911\H,96=1.09591171\H,97=1
 07.85267962\H,98=295.61336394\H,99=1.09496962\H,100=107.43627468\H,101=182.3
 5048592\H,102=1.11279868\H,103=111.56057212\H,104=298.98142686\H,105=1.1003936
 7\H,106=109.31003598\H,107=296.62659052\H,108=1.09689643\H,109=108.48883266\H,110=108.48883266\H,111=108.48883266\H,112=108.48883266\H,113=108.48883266\H,114=108.48883266\H,115=108.48883266\H,116=108.48883266\H,117=108.48883266\H,118=108.48883266\H,119=108.48883266\H,120=108.48883266\H,121=108.48883266\H,122=108.48883266\H,123=108.48883266\H,124=108.48883266\H,125=108.48883266\H,126=108.48883266\H,127=108.48883266\H,128=108.48883266\H,129=108.48883266\H,130=108.48883266\H,131=108.48883266\H,132=108.48883266\H,133=108.48883266\H,134=108.48883266\H,135=108.48883266\H,136=108.48883266\H,137=108.48883266\H,138=108.48883266\H,139=108.48883266\H,140=108.48883266\H,141=108.48883266\H,142=108.48883266\H,143=108.48883266\H,144=108.48883266\H,145=108.48883266\H,146=108.48883266\H,147=108.48883266\H,148=108.48883266\H,149=108.48883266\H,150=108.48883266\H,151=108.48883266\H,152=108.48883266\H,153=108.48883266\H,154=108.48883266\H,155=108.48883266\H,156=108.48883266\H,157=108.48883266\H,158=108.48883266\H,159=108.48883266\H,160=108.48883266\H,161=108.48883266\H,162=108.48883266\H,163=108.48883266\H,164=108.48883266\H,165=108.48883266\H,166=108.48883266\H,167=108.48883266\H,168=108.48883266\H,169=108.48883266\H,170=108.48883266\H,171=108.48883266\H,172=108.48883266\H,173=108.48883266\H,174=108.48883266\H,175=108.48883266\H,176=108.48883266\H,177=108.48883266\H,178=108.48883266\H,179=108.48883266\H,180=108.48883266\H,181=108.48883266\H,182=108.48883266\H,183=108.48883266\H,184=108.48883266\H,185=108.48883266\H,186=108.48883266\H,187=108.48883266\H,188=108.48883266\H,189=108.48883266\H,190=108.48883266\H,191=108.48883266\H,192=108.48883266\H,193=108.48883266\H,194=108.48883266\H,195=108.48883266\H,196=108.48883266\H,197=108.48883266\H,198=108.48883266\H,199=108.48883266\H,200=108.48883266\H,201=108.48883266\H,202=108.48883266\H,203=108.48883266\H,204=108.48883266\H,205=108.48883266\H,206=108.48883266\H,207=108.48883266\H,208=108.48883266\H,209=108.48883266\H,210=108.48883266\H,211=108.48883266\H,212=108.48883266\H,213=108.48883266\H,214=108.48883266\H,215=108.48883266\H,216=108.48883266\H,217=108.48883266\H,218=108.48883266\H,219=108.48883266\H,220=108.48883266\H,221=108.48883266\H,222=108.48883266\H,223=108.48883266\H,224=108.48883266\H,225=108.48883266\H,226=108.48883266\H,227=108.48883266\H,228=108.48883266\H,229=108.48883266\H,230=108.48883266\H,231=108.48883266\H,232=108.48883266\H,233=108.48883266\H,234=108.48883266\H,235=108.48883266\H,236=108.48883266\H,237=108.48883266\H,238=108.48883266\H,239=108.48883266\H,240=108.48883266\H,241=108.48883266\H,242=108.48883266\H,243=108.48883266\H,244=108.48883266\H,245=108.48883266\H,246=108.48883266\H,247=108.48883266\H,248=108.48883266\H,249=108.48883266\H,250=108.48883266\H,251=108.48883266\H,252=108.48883266\H,253=108.48883266\H,254=108.48883266\H,255=108.48883266\H,256=108.48883266\H,257=108.48883266\H,258=108.48883266\H,259=108.48883266\H,260=108.48883266\H,261=108.48883266\H,262=108.48883266\H,263=108.48883266\H,264=108.48883266\H,265=108.48883266\H,266=108.48883266\H,267=108.48883266\H,268=108.48883266\H,269=108.48883266\H,270=108.48883266\H,271=108.48883266\H,272=108.48883266\H,273=108.48883266\H,274=108.48883266\H,275=108.48883266\H,276=108.48883266\H,277=108.48883266\H,278=108.48883266\H,279=108.48883266\H,280=108.48883266\H,281=108.48883266\H,282=108.48883266\H,283=108.48883266\H,284=108.48883266\H,285=108.48883266\H,286=108.48883266\H,287=108.48883266\H,288=108.48883266\H,289=108.48883266\H,290=108.48883266\H,291=108.48883266\H,292=108.48883266\H,293=108.48883266\H,294=108.48883266\H,295=108.48883266\H,296=108.48883266\H,297=108.48883266\H,298=108.48883266\H,299=108.48883266\H,300=108.48883266\H,301=108.48883266\H,302=108.48883266\H,303=108.48883266\H,304=108.48883266\H,305=108.48883266\H,306=108.48883266\H,307=108.48883266\H,308=108.48883266\H,309=108.48883266\H,310=108.48883266\H,311=108.48883266\H,312=108.48883266\H,313=108.48883266\H,314=108.48883266\H,315=108.48883266\H,316=108.48883266\H,317=108.48883266\H,318=108.48883266\H,319=108.48883266\H,320=108.48883266\H,321=108.48883266\H,322=108.48883266\H,323=108.48883266\H,324=108.48883266\H,325=108.48883266\H,326=108.48883266\H,327=108.48883266\H,328=108.48883266\H,329=108.48883266\H,330=108.48883266\H,331=108.48883266\H,332=108.48883266\H,333=108.48883266\H,334=108.48883266\H,335=108.48883266\H,336=108.48883266\H,337=108.48883266\H,338=108.48883266\H,339=108.48883266\H,340=108.48883266\H,341=108.48883266\H,342=108.48883266\H,343=108.48883266\H,344=108.48883266\H,345=108.48883266\H,346=108.48883266\H,347=108.48883266\H,348=108.48883266\H,349=108.48883266\H,350=108.48883266\H,351=108.48883266\H,352=108.48883266\H,353=108.48883266\H,354=108.48883266\H,355=108.48883266\H,356=108.48883266\H,357=108.48883266\H,358=108.48883266\H,359=108.48883266\H,360=108.48883266\H,361=108.48883266\H,362=108.48883266\H,363=108.48883266\H,364=108.48883266\H,365=108.48883266\H,366=108.48883266\H,367=108.48883266\H,368=108.48883266\H,369=108.48883266\H,370=108.48883266\H,371=108.48883266\H,372=108.48883266\H,373=108.48883266\H,374=108.48883266\H,375=108.48883266\H,376=108.48883266\H,377=108.48883266\H,378=108.48883266\H,379=108.48883266\H,380=108.48883266\H,381=108.48883266\H,382=108.48883266\H,383=108.48883266\H,384=108.48883266\H,385=108.48883266\H,386=108.48883266\H,387=108.48883266\H,388=108.48883266\H,389=108.48883266\H,390=108.48883266\H,391=108.48883266\H,392=108.48883266\H,393=108.48883266\H,394=108.48883266\H,395=108.48883266\H,396=108.48883266\H,397=108.48883266\H,398=108.48883266\H,399=108.48883266\H,400=108.48883266\H,401=108.48883266\H,402=108.48883266\H,403=108.48883266\H,404=108.48883266\H,405=108.48883266\H,406=108.48883266\H,407=108.48883266\H,408=108.48883266\H,409=108.48883266\H,410=108.48883266\H,411=108.48883266\H,412=108.48883266\H,413=108.48883266\H,414=108.48883266\H,415=108.48883266\H,416=108.48883266\H,417=108.48883266\H,418=108.48883266\H,419=108.48883266\H,420=108.48883266\H,421=108.48883266\H,422=108.48883266\H,423=108.48883266\H,424=108.48883266\H,425=108.48883266\H,426=108.48883266\H,427=108.48883266\H,428=108.48883266\H,429=108.48883266\H,430=108.48883266\H,431=108.48883266\H,432=108.48883266\H,433=108.48883266\H,434=108.48883266\H,435=108.48883266\H,436=108.48883266\H,437=108.48883266\H,438=108.48883266\H,439=108.48883266\H,440=108.48883266\H,441=108.48883266\H,442=108.48883266\H,443=108.48883266\H,444=108.48883266\H,445=108.48883266\H,446=108.48883266\H,447=108.48883266\H,448=108.48883266\H,449=108.48883266\H,450=108.48883266\H,451=108.48883266\H,452=108.48883266\H,453=108.48883266\H,454=108.48883266\H,455=108.48883266\H,456=108.48883266\H,457=108.48883266\H,458=108.48883266\H,459=108.48883266\H,460=108.48883266\H,461=108.48883266\H,462=108.48883266\H,463=108.48883266\H,464=108.48883266\H,465=108.48883266\H,466=108.48883266\H,467=108.48883266\H,468=108.48883266\H,469=108.48883266\H,470=108.48883266\H,471=108.48883266\H,472=108.48883266\H,473=108.48883266\H,474=108.48883266\H,475=108.48883266\H,476=108.48883266\H,477=108.48883266\H,478=108.48883266\H,479=108.48883266\H,480=108.48883266\H,481=108.48883266\H,482=108.48883266\H,483=108.48883266\H,484=108.48883266\H,485=108.48883266\H,486=108.48883266\H,487=108.48883266\H,488=108.48883266\H,489=108.48883266\H,490=108.48883266\H,491=108.48883266\H,492=108.48883266\H,493=108.48883266\H,494=108.48883266\H,495=108.48883266\H,496=108.48883266\H,497=108.48883266\H,498=108.48883266\H,499=108.48883266\H,500=108.48883266\H,501=108.48883266\H,502=108.48883266\H,503=108.48883266\H,504=108.48883266\H,505=108.4

0=51.65967561\r41=1.0870807\ a41=121.55938923\ d41=178.96285969\r42=1.09706637\ a42=111.09281394\ d42=301.05154685\r43=1.09684321\ a43=111.04674156\ d43=63.19928062\r44=1.09100316\ a44=106.29867176\ d44=182.11052483\r45=1.0910019\ a45=105.51462045\ d45=179.98996195\r46=1.09349221\ a46=110.80096431\ d46=299.60562541\r47=1.09343979\ a47=110.78816576\ d47=60.38063684\r48=1.09619265\ a48=110.78102058\ d48=185.19217416\r49=1.09690811\ a49=111.01300405\ d49=304.76083582\r50=1.09560679\ a50=112.3355118\ d50=65.31784134\r51=1.00766232\ a51=125.4250177\ d51=353.92775081\r52=1.08726347\ a52=120.38394319\ d52=360.23837894\r53=1.08682105\ a53=119.65666465\ d53=180.08867464\r54=1.086735\ a54=119.49758602\ d54=180.09012355\r55=1.08737269\ a55=121.07360768\ d55=179.90277573\\Version=IBM-RS6000-G98RevA.7\ **HF=-1190.3724895**\RMSD=4.154e-09\RMSF=6.075e-05\Dipole=-1.7950044,-0.2770519,-1.8523744\PG=C01 [X(C22H28N2O3)]\ \@

Compound 8 (RINI transition state)CONFORMATIONAL ENERGY, PART 3: GEOMETRY AND STERIC ENERGY
OF FINAL CONFORMATION.

CONNECTED ATOMS

1- 2- 3- 4- 5- 6- 10- 9-

1- 6-

1- 7- 8- 9-

ATTACHED ATOMS

8- 11, 9- 12, 1- 13, 2- 14, 3- 15, 4- 16, 4- 17,

5- 18, 5- 19, 7- 20, 7- 21, 8- 22, 9- 23, 10- 24,

10- 25,

FINAL ATOMIC COORDINATE

ATOM	X	Y	Z	TYPE
C(1)	.08188	-.76571	-.67424	(1)
C(2)	1.51765	-1.22372	-.56707	(2)
C(3)	2.42188	-.54809	.15094	(2)
C(4)	2.02868	.72547	.85691	(1)
C(5)	1.01046	1.51041	.02033	(1)
N(6)	-.05360	.68278	-.54455	(8)
C(7)	-.77448	-1.43234	.42262	(1)
C(8)	-2.22680	-.93511	.39480	(1)
C(9)	-2.28946	.59639	.46321	(1)
C(10)	-1.40992	1.21134	-.62642	(1)
H(11)	-2.79817	-1.37799	1.24300	(5)
H(12)	-3.34177	.94386	.35067	(5)
H(13)	-.30402	-1.06199	-1.67681	(5)
H(14)	1.79487	-2.17060	-1.06085	(5)
H(15)	3.45187	-.92378	.27013	(5)
H(16)	1.60410	.47442	1.85503	(5)
H(17)	2.92991	1.35485	1.03516	(5)
H(18)	1.54190	2.01438	-.82335	(5)
H(19)	.57144	2.32614	.65001	(5)
H(20)	-.33659	-1.21763	1.42434	(5)
H(21)	-.75557	-2.53936	.29752	(5)
H(22)	-2.71988	-1.28518	-.54151	(5)
H(23)	-1.93972	.93986	1.46383	(5)
H(24)	-1.40333	2.32119	-.54636	(5)
H(25)	-1.83471	.97094	-1.62672	(5)

DIELECTRIC CONSTANT = 1.500

BOND LENGTHS AND STRETCHING ENERGY (26 BONDS)

ENERGY = 71.94(KS)(DR)(DR)(1-(CS)(DR)+(7/12)((CS)(DR))**2)

DR = R-RO

CS = 2.550

BOND	LENGTH	R(0)	R(0)-CORR	CORR	ENERGY	E-NEG	MISCEL	KS
C(1)- C(2)	1.5109	1.4990	6.300	.0619				
C(1)- N(6)	1.4606	1.4480	5.300	.0585				
C(1)- C(7)	1.5430	1.5259	4.490	.0905	-.0050	.0062	HY	
C(1)- H(13)	1.1144	1.1110	4.844	.0040	-.0011	.0001	BH	.034
C(2)- C(3)	1.3378	1.3320	7.500	.0177				
C(2)- H(14)	1.1033	1.1010	5.150	.0019				
C(3)- C(4)	1.5083	1.4990	6.300	.0383				
C(3)- H(15)	1.1028	1.1010	5.150	.0012				
C(4)- C(5)	1.5339	1.5218	4.490	.0456	-.0050	.0021	HY	
C(4)- H(16)	1.1134	1.1116	4.694	.0011	-.0004			.014
C(4)- H(17)	1.1136	1.1116	4.694	.0014	-.0004			.014
C(5)- N(6)	1.4616	1.4480	5.300	.0681				
C(5)- H(18)	1.1172	1.1146	4.593	.0022	-.0011	.0037	BH	-.087
C(5)- H(19)	1.1201	1.1183	4.475	.0011	-.0011	.0074	BH	-.205
N(6)- C(10)	1.4580	1.4480	5.300	.0369				
C(7)- C(8)	1.5353	1.5227	4.490	.0499	-.0020			
C(7)- H(20)	1.1141	1.1116	4.694	.0022	-.0004			.014

S140

```

C( 7)- H( 21) 1.1142 1.1116 4.694 .0024 -.0004 .014
C( 8)- C( 9) 1.5343 1.5227 4.490 .0422 -.0020
C( 8)- H( 11) 1.1145 1.1120 4.680 .0020
C( 8)- H( 22) 1.1146 1.1120 4.680 .0023
C( 9)- C( 10) 1.5294 1.5197 4.490 .0296 -.0050
C( 9)- H( 12) 1.1139 1.1116 4.694 .0018 -.0004 .014
C( 9)- H( 23) 1.1142 1.1116 4.694 .0024 -.0004 .014
C( 10)- H( 24) 1.1127 1.1117 4.688 .0003 -.0011 .0008 BH .008
C( 10)- H( 25) 1.1130 1.1111 4.709 .0012 -.0011 .0002 BH .029

```

NON-BONDED DISTANCES, VDW AND EPR ENERGY (223 PAIRS)

```

E(VDW) = KV*(1.84(10**5)EXP(-12.00/P) - 2.25(P**6))
E(EPR) = C*KV*(1.84(10**5)EXP(-12.00/Q) - 2.25(Q**6))
E(HBD) = EP1-EP2*COS(THETA)*RTH/RTH0
          EP1 = KHB*1.84(10**5)*EXP(-12.0/P)
          EP2 = KHB*2.25(P**6)

```

IF P > 3.020, THEN,

```

E(VDW) = KV(192.270)(P**2)
E(HBD) = EP1-EP2*COS(THETA)*RTH/RTH0
          EP1 = KHB*(192.270*P**2+1706.96)
          EP2 = KHB*1706.96

```

WHERE RV = RVDW(I) + RVDW(K)

KV = SQRT(EPS(I)*EPS(K))

KHB = EPS/DIELEC FOR HYDROGEN BOND

P = (RV/R) OR (RV/R#)

C = SCALE FACTOR

Q = RV/R, WHERE R IS MODIFIED DISTANCE

THETA = ANGLE H-X-Y IN HYDROGEN BOND X-H...Y

RTH = BOND LENGTH X-H IN X-H...Y

RTH0 = NATURAL BOND LENGTH X-H

IN THE VDW CALCULATIONS THE HYDROGEN ATOMS ARE RELOCATED
SO THAT THE ATTACHED HYDROGEN DISTANCE IS REDUCED BY .923

IN THE VDW CALCULATIONS THE DEUTERIUM ATOMS ARE RELOCATED
SO THAT THE ATTACHED DEUTERIUM DISTANCE IS REDUCED BY .923

** INTERACTIONS OF LESS THAN 0.1 KCAL/MOL ARE NOT PRINTED **

ATOM PAIR	R	R#	RV	KV	ENERGY
C(1), C(4)	2.8910		4.080	.0270	.5278 1,4
C(1), C(9)	2.9618		4.080	.0270	.4033 1,4
C(1), H(22)	2.8526	2.8148	3.560	.0230	.1088 1,4
C(1), H(25)	2.7562	2.7196	3.560	.0230	.1815 1,4
C(2), C(5)	2.8421		4.000	.0389	.7379 1,4
C(2), H(20)	2.7210	2.6887	3.580	.0335	.3310 1,4
C(2), H(21)	2.7651	2.7299	3.580	.0335	.2708 1,4
C(3), N(6)	2.8507		3.890	.0491	.6563 1,4
C(3), H(18)	2.8792	2.8362	3.580	.0335	.1533 1,4
C(5), H(24)	2.6086	2.5852	3.560	.0230	.3422 1,4
N(6), C(8)	2.8675		3.970	.0341	.5389 1,4
N(6), H(20)	2.7510	2.7118	3.550	.0293	.2316 1,4
N(6), H(23)	2.7672	2.7282	3.550	.0293	.2130 1,4
C(7), C(10)	2.9143		4.080	.0270	.4837 1,4
C(7), H(23)	2.8406	2.8024	3.560	.0230	.1168 1,4
C(8), H(13)	2.8293	2.7930	3.560	.0230	.1231 1,4
C(8), H(25)	2.8059	2.7686	3.560	.0230	.1406 1,4
C(9), H(20)	2.8334	2.7956	3.560	.0230	.1213 1,4
C(10), H(13)	2.7376	2.7021	3.560	.0230	.1980 1,4
C(10), H(19)	2.6073	2.5837	3.560	.0230	.3445 1,4
C(10), H(22)	2.8206	2.7823	3.560	.0230	.1306 1,4
H(11), H(12)	2.5461	2.4573	3.240	.0200	.1740 1,4
H(11), H(20)	2.4735	2.3924	3.240	.0200	.2444 1,4
H(11), H(21)	2.5328	2.4452	3.240	.0200	.1857 1,4
H(11), H(23)	2.4816	2.3999	3.240	.0200	.2353 1,4
H(12), H(22)	2.4802	2.3987	3.240	.0200	.2366 1,4
H(12), H(24)	2.5415	2.4532	3.240	.0200	.1779 1,4

S141

H(12), H(25)	2.4864	2.4037	3.240	.0200	.2308	1,4
H(13), H(14)	2.4523	2.3763	3.240	.0200	.2650	1,4
H(13), H(21)	2.5069	2.4230	3.240	.0200	.2088	1,4
H(13), H(25)	2.5453	2.5400	3.240	.0200	.1083	
H(14), H(15)	2.4641	2.3774	3.240	.0200	.2636	1,4
H(15), H(17)	2.4596	2.3845	3.240	.0200	.2543	1,4
H(16), H(19)	2.4387	2.3622	3.240	.0200	.2842	1,4
H(17), H(18)	2.4116	2.3375	3.240	.0200	.3206	1,4
H(17), H(19)	2.5796	2.4856	3.240	.0200	.1489	1,4
H(19), H(24)	2.3089	2.3171	3.240	.0200	.3535	
H(21), H(22)	2.4770	2.3955	3.240	.0200	.2406	1,4
H(23), H(24)	2.4973	2.4137	3.240	.0200	.2191	1,4

BOND ANGLES, BENDING AND STRETCH-BEND ENERGIES (51 ANGLES)

$$EB = 0.021914(KB)(DT)(DT)(1+CF*DT+QF*DT**2+PF*DT**3+SF*DT**4)$$

$$DT = THETA-TZERO$$

$$CF = -1400.000E-5$$

$$QF = 5.600E-5$$

$$PF = -.070E-5$$

$$SF = .022E-6$$

$$ESB(J) = 2.51124(KSB(J))(DT)(DR1+DR2)$$

$$DR(I) = R(I) - R0(I)$$

$$EBDBD = -0.02191418(KBB1)(DT1)(KBB2)(DT2)$$

A T O M S		THETA	TZERO	KB	EB	KSB	ESB	
C(2)- C(1)- N(6)	112.488	110.740	1.045	.0682	.13	.0139	C	
C(2)- C(1)- C(7)	110.244	109.800	.540	.0023	.13	.0042		
C(2)- C(1)- H(13)	108.198	109.500	.550	.0208	.08	-.0040		
N(6)- C(1)- C(7)	108.292	108.000	.780	.0014	.13	.0028		
N(6)- C(1)- H(13)	108.146	109.300	.820	.0243	.08	-.0037		
C(7)- C(1)- H(13)	109.419	109.800	.590	.0019	.08	-.0016		
C(1)- C(2)- C(3)	121.823	122.300		.13	-.0027			
IN-PLN 1- 2- 3	121.844	122.300	.470	.0022				
OUT-PL 2- 14- 2	1.043	.110	.0027					
C(1)- C(2)- H(14)	117.853	117.500		.08	.0010			
IN-PLN 1- 2- 14	117.876	117.500	.490	.0015				
OUT-PL 2- 3- 2	.860	.200	.0033					
C(3)- C(2)- H(14)	120.253	120.000		.08	.0004			
IN-PLN 3- 2- 14	120.280	120.000	.490	.0008				
OUT-PL 2- 1- 2	.761	.100	.0013					
C(2)- C(3)- C(4)	120.096	122.300		.13	-.0108			
IN-PLN 2- 3- 4	120.106	122.300	.470	.0511				
OUT-PL 3- 15- 3	.748	.110	.0014					
C(2)- C(3)- H(15)	121.147	120.000		.08	.0018			
IN-PLN 2- 3- 15	121.162	120.000	.490	.0143				
OUT-PL 3- 4- 3	.546	.100	.0007					
C(4)- C(3)- H(15)	118.720	117.500		.08	.0027			
IN-PLN 4- 3- 15	118.732	117.500	.490	.0160				
OUT-PL 3- 2- 3	.615	.200	.0017					
C(3)- C(4)- C(5)	110.479	110.600	.540	.0002	.13	-.0008		
C(3)- C(4)- H(16)	109.186	109.310	.550	.0002	.08	-.0003		
C(3)- C(4)- H(17)	109.948	109.310	.550	.0049	.08	.0015		
C(5)- C(4)- H(16)	110.561	109.310	.590	.0199	.08	.0035		
C(5)- C(4)- H(17)	109.592	109.310	.590	.0010	.08	.0008		
H(16)- C(4)- H(17)	107.011	107.600	.550	.0042				
C(4)- C(5)- N(6)	113.847	111.000	.780	.1331	.13	.0239		
C(4)- C(5)- H(18)	109.083	109.310	.590	.0007	.08	-.0007		
C(4)- C(5)- H(19)	109.041	109.310	.590	.0009	.08	-.0007		
N(6)- C(5)- H(18)	108.052	109.300	.820	.0285	.08	-.0041		
N(6)- C(5)- H(19)	110.139	109.300	.820	.0125	.08	.0026		
H(18)- C(5)- H(19)	106.406	107.600	.550	.0175				
C(1)- N(6)- C(5)	121.894	107.200	.720	2.7430	.05	.0483		
C(1)- N(6)- C(10)	116.157	107.200	.720	1.1124	.05	.0254		
C(5)- N(6)- C(10)	119.582	107.200	.720	2.0185	.05	.0366		
C(1)- C(7)- C(8)	111.851	111.000	.670	.0105	.13	.0083		
C(1)- C(7)- H(20)	109.739	109.310	.590	.0024	.08	.0017		
C(1)- C(7)- H(21)	109.877	109.310	.590	.0041	.08	.0023		
C(8)- C(7)- H(20)	109.006	109.310	.590	.0012	.08	-.0009		
C(8)- C(7)- H(21)	109.621	109.310	.590	.0012	.08	.0010		

S142

```

H( 20)- C( 7)- H( 21) 106.603 107.600 .550 .0121
C( 7)- C( 8)- C( 9) 111.167 111.000 .670 .0004 .13 .0013
C( 7)- C( 8)- H( 11) 110.028 109.310 .590 .0066 .08 .0022
C( 7)- C( 8)- H( 22) 109.388 109.310 .590 .0001 .08 .0002
C( 9)- C( 8)- H( 11) 109.986 109.310 .590 .0059 .08 .0019
C( 9)- C( 8)- H( 22) 109.444 109.310 .590 .0002 .08 .0004
H( 11)- C( 8)- H( 22) 106.722 107.600 .550 .0094
C( 8)- C( 9)- C( 10) 110.249 111.000 .670 .0084 .13 -.0052
C( 8)- C( 9)- H( 12) 110.209 109.310 .590 .0103 .08 .0025
C( 8)- C( 9)- H( 23) 109.567 109.310 .590 .0009 .08 .0007
C( 10)- C( 9)- H( 12) 110.236 109.310 .590 .0109 .08 .0022
C( 10)- C( 9)- H( 23) 109.594 109.310 .590 .0010 .08 .0007
H( 12)- C( 9)- H( 23) 106.924 107.600 .550 .0056
N( 6)- C( 10)- C( 9) 110.440 111.000 .780 .0054 .13 -.0036
N( 6)- C( 10)- H( 24) 110.612 109.300 .820 .0304 .08 .0029
N( 6)- C( 10)- H( 25) 109.099 109.300 .820 .0007 .08 -.0005
C( 9)- C( 10)- H( 24) 110.682 109.310 .590 .0239 .08 .0029
C( 9)- C( 10)- H( 25) 109.509 109.310 .590 .0005 .08 .0005
H( 24)- C( 10)- H( 25) 106.400 107.600 .550 .0177

```

DIHEDRAL ANGLES, TORSIONAL ENERGY (ET) (79 ANGLES)

$$ET = (V1/2)(1+\cos(W)) + (V2/2)(1-\cos(2W)) + (V3/2)(1+\cos(3W))$$

$$ETS = -11.995 \cdot (R-R0) \cdot ((KTS1/2)(1+\cos(W)) + (KTS2/2)(1-\cos(2W)) + (KTS3/2)(1+\cos(3W)))$$

SIGN OF ANGLE A-B-C-D : WHEN LOOKING THROUGH B TOWARD C,
IF D IS COUNTERCLOCKWISE FROM A, NEGATIVE.

A T O M S				OMEGA	V1	V2	V3	ET	KTS3	ETS
C(1)	C(2)	C(3)	C(4)	-1.4	-.300	9.500	.000	-.294		
C(1)	C(2)	C(3)	H(15)	176.4	.000	10.000	.000	.040		
C(1)	N(6)	C(5)	C(4)	-19.0	.958	-.155	.766	1.507	.061	-.008
C(1)	N(6)	C(5)	H(18)	102.3	.072	-.012	.563	.468	.061	-.008
C(1)	N(6)	C(5)	H(19)	-141.8	.072	-.012	.563	.402	.061	-.007
C(1)	N(6)	C(10)	C(9)	58.8	.958	-.155	.766	.615	.061	.000
C(1)	N(6)	C(10)	H(24)	-178.4	.072	-.012	.563	.001	.061	.000
C(1)	N(6)	C(10)	H(25)	-61.6	.072	-.012	.563	.045	.061	.000
C(1)	C(7)	C(8)	C(9)	-53.8	.185	.170	.520	.271	.059	.000
C(1)	C(7)	C(8)	H(11)	-175.9	.000	.000	.280	.003	.059	.000
C(1)	C(7)	C(8)	H(22)	67.2	.000	.000	.280	.010	.059	.000
C(2)	C(1)	N(6)	C(5)	-17.1	.000	.000	.000	.000	.061	-.007 C
C(2)	C(1)	N(6)	C(10)	-179.6	.000	.000	.000	.000	.061	.000 C
C(2)	C(1)	C(7)	C(8)	177.0	.200	-.200	1.300	.008	.059	.000
C(2)	C(1)	C(7)	H(20)	55.9	.000	.000	.500	.006	.059	.000
C(2)	C(1)	C(7)	H(21)	-61.1	.000	.000	.500	.000	.059	.000
C(2)	C(3)	C(4)	C(5)	-35.7	-.700	-.200	-.550	-.897		
C(2)	C(3)	C(4)	H(16)	86.1	.000	.000	-.090	-.036		
C(2)	C(3)	C(4)	H(17)	-156.8	.000	.000	-.090	-.029		
C(3)	C(2)	C(1)	N(6)	28.9	.000	.000	.000	.000		C
C(3)	C(2)	C(1)	C(7)	-92.1	-.700	-.200	-.550	-.842		
C(3)	C(2)	C(1)	H(13)	148.3	.000	.000	-.090	-.049		
C(3)	C(4)	C(5)	N(6)	44.5	.000	.000	.180	.028	.059	-.001 C
C(3)	C(4)	C(5)	H(18)	-76.2	.000	.000	.500	.085	.059	-.001
C(3)	C(4)	C(5)	H(19)	168.0	.000	.000	.500	.048	.059	-.001
C(4)	C(3)	C(2)	H(14)	-178.3	.000	10.000	.000	.009		
C(4)	C(5)	N(6)	C(10)	142.9	.958	-.155	.766	.563	.061	-.007
C(5)	C(4)	C(3)	H(15)	146.5	.000	.000	.010	.006	.270	-.018
C(5)	N(6)	C(1)	C(7)	105.0	.958	-.155	.766	.864	.061	-.008
C(5)	N(6)	C(1)	H(13)	-136.6	.072	-.012	.563	.468	.061	-.008
C(5)	N(6)	C(10)	C(9)	-104.1	.958	-.155	.766	.857	.061	-.006
C(5)	N(6)	C(10)	H(24)	18.8	.072	-.012	.563	.506	.061	-.006
C(5)	N(6)	C(10)	H(25)	135.5	.072	-.012	.563	.480	.061	-.006
N(6)	C(1)	C(2)	H(14)	-154.2	.000	.000	.000	.000	.270	-.015 C
N(6)	C(1)	C(7)	C(8)	53.5	-.302	.696	.499	.223	.059	.000
N(6)	C(1)	C(7)	H(20)	-67.6	.000	.000	.374	.015	.059	.000
N(6)	C(1)	C(7)	H(21)	175.5	.000	.000	.374	.005	.059	.000
N(6)	C(5)	C(4)	H(16)	-76.4	.000	.000	.374	.065	.059	-.001

S143

```

N( 6) C( 5) C( 4) H( 17) 165.8 .000 .000 .374 .049 .059 -.001
N( 6) C( 10) C( 9) C( 8) -53.9 -.302 .696 .499 .227 .059 .000
N( 6) C( 10) C( 9) H( 12) -175.8 .000 .000 .374 .005 .059 .000
N( 6) C( 10) C( 9) H( 23) 66.8 .000 .000 .374 .012 .059 .000
C( 7) C( 1) C( 2) H( 14) 84.8 .000 .000 .010 .004 .270 -.014
C( 7) C( 1) N( 6) C( 10) -57.5 .958 -.155 .766 .630 .061 .000
C( 7) C( 8) C( 9) C( 10) 53.1 .185 .170 .520 .274 .059 .000
C( 7) C( 8) C( 9) H( 12) 175.0 .000 .000 .280 .005 .059 .000
C( 7) C( 8) C( 9) H( 23) -67.6 .000 .000 .280 .011 .059 .000
C( 8) C( 7) C( 1) H( 13) -64.2 .000 .000 .280 .003 .059 .000
C( 8) C( 9) C( 10) H( 24) -176.7 .000 .000 .280 .002 .059 .000
C( 8) C( 9) C( 10) H( 25) 66.3 .000 .000 .280 .008 .059 .000
C( 9) C( 8) C( 7) H( 20) 67.7 .000 .000 .280 .011 .059 .000
C( 9) C( 8) C( 7) H( 21) -175.9 .000 .000 .280 .003 .059 .000
C( 10) N( 6) C( 1) H( 13) 61.0 .072 -.012 .563 .045 .061 .000
C( 10) N( 6) C( 5) H( 18) -95.8 .072 -.012 .563 .386 .061 -.006
C( 10) N( 6) C( 5) H( 19) 20.0 .072 -.012 .563 .490 .061 -.007
C( 10) C( 9) C( 8) H( 11) 175.2 .000 .000 .280 .004 .059 .000
C( 10) C( 9) C( 8) H( 22) -67.9 .000 .000 .280 .012 .059 .000
H( 11) C( 8) C( 7) H( 20) -54.4 .000 .000 .238 .005 .059 .000
H( 11) C( 8) C( 7) H( 21) 62.0 .000 .000 .238 .001 .059 .000
H( 11) C( 8) C( 9) H( 12) -62.9 .000 .000 .238 .001 .059 .000
H( 11) C( 8) C( 9) H( 23) 54.5 .000 .000 .238 .005 .059 .000
H( 12) C( 9) C( 8) H( 22) 54.0 .000 .000 .238 .006 .059 .000
H( 12) C( 9) C( 10) H( 24) 61.4 .000 .000 .238 .000 .059 .000
H( 12) C( 9) C( 10) H( 25) -55.6 .000 .000 .238 .003 .059 .000
H( 13) C( 1) C( 2) H( 14) -34.8 .000 .000 .580 .218 .270 -.014
H( 13) C( 1) C( 7) H( 20) 174.7 .000 .000 .238 .005 .059 .000
H( 13) C( 1) C( 7) H( 21) 57.8 .000 .000 .238 .001 .059 .000
H( 14) C( 2) C( 3) H( 15) -.5 .000 11.500 .000 .001
H( 15) C( 3) C( 4) H( 16) -91.7 .000 .000 .580 .316 .270 -.016
H( 15) C( 3) C( 4) H( 17) 25.4 .000 .000 .580 .359 .270 -.019
H( 16) C( 4) C( 5) H( 18) 162.8 .000 .000 .238 .045 .059 -.002
H( 16) C( 4) C( 5) H( 19) 47.0 .000 .000 .238 .027 .059 -.001
H( 17) C( 4) C( 5) H( 18) 45.1 .000 .000 .238 .034 .059 -.001
H( 17) C( 4) C( 5) H( 19) -70.7 .000 .000 .238 .018 .059 -.001
H( 20) C( 7) C( 8) H( 22) -171.3 .000 .000 .238 .012 .059 .000
H( 21) C( 7) C( 8) H( 22) -54.9 .000 .000 .238 .004 .059 .000
H( 22) C( 8) C( 9) H( 23) 171.4 .000 .000 .238 .012 .059 .000
H( 23) C( 9) C( 10) H( 24) -56.0 .000 .000 .238 .003 .059 .000
H( 23) C( 9) C( 10) H( 25) -173.0 .000 .000 .238 .008 .059 .000

```

DIPOLE-DIPOLE INTERACTION ENERGY (DIELECTRIC CONSTANT = 1.50)

$$E = 14.388 * MU1 * MU2 * (\cos X - 3 * \cos A * \cos B) / (R12^3 * \text{DIELC})$$

MU1 = BOND MOM OF BOND 1

MU2 = BOND MOM OF BOND 2

R12 = DISTANCE BETWEEN MID-POINTS OF TWO BONDS.

(ENERGIES LESS THAN 0.2 KCAL/MOL ARE NOT PRINTED.)

BOND(1)	MU1	BOND(2)	MU2	R12	E
C(1)- C(2)	.900	+ C(3)- C(4)	-.900	2.1144	1.0392
C(1)- C(2)	.900	+ C(3)- H(15)	-.600	2.3076	.5333
C(1)- C(2)	.900	+ C(5)- N(6)	.680	2.1460	-.7103
C(1)- C(2)	.900	+ N(6)- C(10)	-.680	2.4733	-.4390
C(1)- N(6)	.680	+ C(2)- H(14)	-.600	2.3409	-.3039
C(1)- N(6)	.680	+ C(3)- C(4)	-.900	2.4790	-.3478
C(2)- H(14)	-.600	+ C(3)- C(4)	-.900	2.2913	.5323
C(2)- H(14)	-.600	+ C(3)- H(15)	-.600	1.9009	.6337
C(3)- C(4)	-.900	+ C(5)- N(6)	.680	2.1574	.6305

=====

NORMAL MODE VIBRATIONAL ANALYSIS

=====

Molecular Shape : ASYMMETRIC ROTOR WITH KAPPA = -.658056
Symmetry Point Group : C1

Symmetry Number : 1
Chirality : yes

0 FUNDAMENTAL NORMAL VIBRATIONAL FREQUENCIES
(THEORETICALLY 69 VALUES)

Frequency : in 1/cm

A(i) : IR intensity (vs,s,m,w,vw,-- or in 10**6 cm/mole)

A(i) = -- : IR inactive

no	Frequency	Symmetry	A(i)
1.	3057.7	(A)	m
2.	3042.8	(A)	w
3.	2942.4	(A)	m
4.	2937.7	(A)	m
5.	2937.1	(A)	m
6.	2932.5	(A)	m
7.	2929.5	(A)	m
8.	2926.0	(A)	m
9.	2893.0	(A)	m
10.	2886.6	(A)	w
11.	2884.9	(A)	m
12.	2884.0	(A)	m
13.	2877.7	(A)	m
14.	2868.1	(A)	m
15.	2827.5	(A)	m
16.	1678.6	(A)	w
17.	1593.0	(A)	vw
18.	1557.0	(A)	w
19.	1552.0	(A)	w
20.	1495.6	(A)	w
21.	1466.9	(A)	w
22.	1461.4	(A)	vw
23.	1458.1	(A)	w
24.	1450.3	(A)	w
25.	1437.5	(A)	w
26.	1428.4	(A)	w
27.	1403.7	(A)	w
28.	1393.3	(A)	w
29.	1383.1	(A)	w
30.	1373.0	(A)	w
31.	1355.1	(A)	m
32.	1330.3	(A)	w
33.	1304.3	(A)	w
34.	1249.6	(A)	w
35.	1229.5	(A)	w
36.	1217.1	(A)	w
37.	1208.1	(A)	w
38.	1187.5	(A)	w
39.	1178.3	(A)	w
40.	1153.6	(A)	w
41.	1092.7	(A)	w
42.	1052.4	(A)	w
43.	1045.7	(A)	w
44.	1027.5	(A)	w
45.	1006.9	(A)	w
46.	984.9	(A)	w
47.	951.1	(A)	vw
48.	928.6	(A)	w
49.	918.5	(A)	w
50.	892.4	(A)	w
51.	851.7	(A)	w
52.	832.5	(A)	w
53.	826.0	(A)	w
54.	798.9	(A)	w
55.	722.7	(A)	w
56.	669.2	(A)	w

57.	634.3	(A)	m
58.	551.8	(A)	w
59.	496.7	(A)	w
60.	454.5	(A)	w
61.	418.3	(A)	w
62.	379.1	(A)	w
63.	365.6	(A)	w
64.	356.8	(A)	w
65.	258.1	(A)	w
66.	235.4	(A)	w
67.	177.9	(A)	vw
68.	-111.8	(imag)	w
69.	95.8	(A)	vw
70.	(.0)	(t/r)	
71.	(.0)	(t/r)	
72.	(.0)	(t/r)	
73.	(.0)	(t/r)	
74.	(.0)	(t/r)	
75.	(.0)	(t/r)	

=====

STATISTICAL THERMODYNAMICS ANALYSIS

=====

Structure name : RINI
 Temperature : 298.16 K
 Symmetry number : 1
 Optical isomers : 2
 Zero Point Energy : 139.236 Kcal/mol

	ENERGY (Kcal/mol)	ENTHALPY (Kcal/mol)	ENTROPY (eu)	FREE ENERGY (Kcal/mol)	HEAT CAPACITY (cal/mol/deg)
Translational	.889	1.481	40.641	-10.636	4.967
Rotational	.889	.889	29.215	-7.822	2.980
Vibrational	142.749%	142.749%	18.897*	137.114%	29.223*
Potential	25.629#	25.629#	.000	25.629#	.000
Mixing	.000	.000	1.377	-.411	.000
Total	170.155	170.747	90.130	143.874	37.171

Enthalpy Function (H-Ho)/T = 19.73 cal/mol/deg
 Free Energy Function -(G-Ho)/T = 70.40 cal/mol/deg

% Includes zero point energy (ZPE).
 * Excludes contribution from frequencies lower than 40 (1/cm).
 # Includes steric energy (SE).
 Internal rotation contributions are not considered

This structure has 1 imaginary frequencies,
 0 free internal rotation (fir) frequencies
 (>= 0,< 10 /cm),
 0 restricted internal rotation (rir) frequencies
 (>= 10,< 40 /cm),
 6 zero frequencies, and
 68 real frequencies.

FINAL STERIC ENERGY IS 25.6285 KCAL/MOL.

COMPRESSION .5670
 BENDING 6.4830
 BEND-BEND -.5273
 STRETCH-BEND .1614
 VANDERWAALS
 1,4 ENERGY 9.8184
 OTHER -1.1088

TORSIONAL 8.7137
 TORSION-STRETCH -.1980

DIPOLE-DIPOLE 1.7193
 CHARGE-DIPOLE .0000
 CHARGE-CHARGE .0000

COORDINATES TRANSLATED TO NEW ORIGIN WHICH IS CENTER OF MASS

C(1)	.08188	-.76571	-.67424	(1)
C(2)	1.51765	-1.22372	-.56707	(2)
C(3)	2.42188	-.54809	.15094	(2)
C(4)	2.02868	.72547	.85691	(1)
C(5)	1.01046	1.51041	.02033	(1)
N(6)	-.05360	.68278	-.54455	(8)
C(7)	-.77448	-1.43234	.42262	(1)
C(8)	-2.22680	-.93511	.39480	(1)
C(9)	-2.28946	.59639	.46321	(1)
C(10)	-1.40992	1.21134	-.62642	(1)
H(11)	-2.79817	-1.37799	1.24300	(5)
H(12)	-3.34177	.94386	.35067	(5)
H(13)	-.30402	-1.06199	-1.67681	(5)
H(14)	1.79487	-2.17060	-1.06085	(5)
H(15)	3.45187	-.92378	.27013	(5)
H(16)	1.60410	.47442	1.85503	(5)
H(17)	2.92991	1.35485	1.03516	(5)
H(18)	1.54190	2.01438	-.82335	(5)
H(19)	.57144	2.32614	.65001	(5)
H(20)	-.33659	-1.21763	1.42434	(5)
H(21)	-.75557	-2.53936	.29752	(5)
H(22)	-2.71988	-1.28518	-.54151	(5)
H(23)	-1.93972	.93986	1.46383	(5)
H(24)	-1.40333	2.32119	-.54636	(5)
H(25)	-1.83471	.97094	-1.62672	(5)

MOMENT OF INERTIA WITH THE PRINCIPAL AXES

(1) UNIT = 10**(-39) GM*CM**2
 IX= 35.9838 IY= 71.6980 IZ= 90.1507

(2) UNIT = AU A**2
 IX= 216.7230 IY= 431.8228 IZ= 542.9596

DIPOLE MOMENT = .616 D

COMPONENTS WITH PRINCIPAL AXES

X = .4532 Y = -.2706 Z = -.3180

Compound 8 (conformer 1)CONFORMATIONAL ENERGY, PART 3: GEOMETRY AND STERIC ENERGY
OF FINAL CONFORMATION.

CONNECTED ATOMS

1- 2- 3- 4- 5- 6- 10- 9-

1- 6-

1- 7- 8- 9-

ATTACHED ATOMS

8- 11, 9- 12, 1- 13, 2- 14, 3- 15, 4- 16, 4- 17,

5- 18, 5- 19, 7- 20, 7- 21, 8- 22, 9- 23, 10- 24,

10- 25,

FINAL ATOMIC COORDINATE

ATOM	X	Y	Z	TYPE
C(1)	-.07481	-.79329	.59200	(1)
C(2)	-1.48072	-1.30125	.38426	(2)
C(3)	-2.47553	-.53251	-.07666	(2)
C(4)	-2.26951	.92046	-.40844	(1)
C(5)	-.77936	1.26288	-.51932	(1)
N(6)	-.02395	.67195	.58294	(8)
C(7)	.85655	-1.39153	-.48414	(1)
C(8)	2.28920	-.86283	-.35744	(1)
C(9)	2.29912	.66802	-.33496	(1)
C(10)	1.33544	1.18875	.73360	(1)
H(11)	2.91456	-1.23915	-1.19952	(5)
H(12)	3.33002	1.03909	-.13314	(5)
H(13)	.26506	-1.14094	1.59531	(5)
H(14)	-1.67612	-2.36050	.62528	(5)
H(15)	-3.49141	-.94725	-.19320	(5)
H(16)	-2.78316	1.16669	-1.36528	(5)
H(17)	-2.74469	1.53915	.38656	(5)
H(18)	-.66441	2.37022	-.50890	(5)
H(19)	-.37650	.90726	-1.50663	(5)
H(20)	.46752	-1.16242	-1.50177	(5)
H(21)	.86524	-2.50262	-.39794	(5)
H(22)	2.74617	-1.25135	.58204	(5)
H(23)	2.00949	1.06193	-1.33534	(5)
H(24)	1.31966	2.30134	.72456	(5)
H(25)	1.71822	.89916	1.73803	(5)

DIELECTRIC CONSTANT = 1.500

BOND LENGTHS AND STRETCHING ENERGY (26 BONDS)

ENERGY = 71.94(KS)(DR)(DR)(1-(CS)(DR)+(7/12)((CS)(DR))**2)

DR = R-RO

CS = 2.550

BOND	LENGTH	R(0)	R(0)-CORR	CORR	ENERGY	E-NEG	MISCEL	KS
C(1)- C(2)	1.5092	1.4990	6.300	.0462				
C(1)- N(6)	1.4662	1.4480	5.300	.1200				
C(1)- C(7)	1.5438	1.5253	4.490	.1059	-.0050	.0056	HY	
C(1)- H(13)	1.1149	1.1109	4.845	.0055	-.0011	.0000	BH	.035
C(2)- C(3)	1.3390	1.3320	7.500	.0263				
C(2)- H(14)	1.1038	1.1010	5.150	.0028				
C(3)- C(4)	1.5045	1.4990	6.300	.0137				
C(3)- H(15)	1.1035	1.1010	5.150	.0022				
C(4)- C(5)	1.5330	1.5201	4.490	.0517	-.0050	.0004	HY	
C(4)- H(16)	1.1136	1.1116	4.694	.0013	-.0004			.014
C(4)- H(17)	1.1138	1.1116	4.694	.0017	-.0004			.014
C(5)- N(6)	1.4611	1.4480	5.300	.0633				
C(5)- H(18)	1.1133	1.1113	4.702	.0014	-.0011	.0004	BH	.022
C(5)- H(19)	1.1241	1.1234	4.310	.0002	-.0011	.0125	BH	-.370
N(6)- C(10)	1.4621	1.4480	5.300	.0731				
C(7)- C(8)	1.5323	1.5227	4.490	.0293	-.0020			
C(7)- H(20)	1.1133	1.1116	4.694	.0010	-.0004			.014

S148

```

C( 7)- H( 21) 1.1145 1.1116 4.694 .0028 -.0004 .014
C( 8)- C( 9) 1.5310 1.5227 4.490 .0220 -.0020
C( 8)- H( 11) 1.1144 1.1120 4.680 .0019
C( 8)- H( 22) 1.1146 1.1120 4.680 .0023
C( 9)- C( 10) 1.5302 1.5197 4.490 .0350 -.0050
C( 9)- H( 12) 1.1141 1.1116 4.694 .0021 -.0004 .014
C( 9)- H( 23) 1.1135 1.1116 4.694 .0012 -.0004 .014
C( 10)- H( 24) 1.1127 1.1112 4.708 .0008 -.0011 .0003 BH .028
C( 10)- H( 25) 1.1132 1.1109 4.715 .0018 -.0011 .0000 BH .035

```

NON-BONDED DISTANCES, VDW AND EPR ENERGY (223 PAIRS)

```

E(VDW) = KV*(1.84(10**5)EXP(-12.00/P) - 2.25(P**6))
E(EPR) = C*KV*(1.84(10**5)EXP(-12.00/Q) - 2.25(Q**6))
E(HBD) = EP1-EP2*COS(THETA)*RTH/RTH0
          EP1 = KHB*1.84(10**5)*EXP(-12.0/P)
          EP2 = KHB*2.25(P**6)

```

IF P > 3.020, THEN,

```

E(VDW) = KV(192.270)(P**2)
E(HBD) = EP1-EP2*COS(THETA)*RTH/RTH0
          EP1 = KHB*(192.270*P**2+1706.96)
          EP2 = KHB*1706.96

```

WHERE RV = RVDW(I) + RVDW(K)

KV = SQRT(EPS(I)*EPS(K))

KHB = EPS/DIELEC FOR HYDROGEN BOND

P = (RV/R) OR (RV/R#)

C = SCALE FACTOR

Q = RV/R, WHERE R IS MODIFIED DISTANCE

THETA = ANGLE H-X-Y IN HYDROGEN BOND X-H...Y

RTH = BOND LENGTH X-H IN X-H...Y

RTH0 = NATURAL BOND LENGTH X-H

IN THE VDW CALCULATIONS THE HYDROGEN ATOMS ARE RELOCATED
SO THAT THE ATTACHED HYDROGEN DISTANCE IS REDUCED BY .923

IN THE VDW CALCULATIONS THE DEUTERIUM ATOMS ARE RELOCATED
SO THAT THE ATTACHED DEUTERIUM DISTANCE IS REDUCED BY .923

** INTERACTIONS OF LESS THAN 0.1 KCAL/MOL ARE NOT PRINTED **

ATOM PAIR	R	R#	RV	KV	ENERGY
C(1), C(4)	2.9588		4.080	.0270	.4080 1,4
C(1), C(9)	2.9377		4.080	.0270	.4425 1,4
C(1), H(19)	2.7179	2.6809	3.560	.0230	.2197 1,4
C(1), H(22)	2.8579	2.8197	3.560	.0230	.1057 1,4
C(1), H(25)	2.7190	2.6819	3.560	.0230	.2186 1,4
C(2), C(5)	2.8077		4.000	.0389	.8407 1,4
C(2), H(20)	2.7152	2.6825	3.580	.0335	.3409 1,4
C(2), H(21)	2.7493	2.7144	3.580	.0335	.2924 1,4
C(3), N(6)	2.8100		3.890	.0491	.7754 1,4
C(3), H(19)	2.9195	2.8744	3.580	.0335	.1217 1,4
C(5), C(7)	3.1182		4.080	.0270	.2118 1,4
C(5), C(9)	3.1408		4.080	.0270	.1915 1,4
C(5), H(24)	2.6517	2.6206	3.560	.0230	.2916 1,4
N(6), C(8)	2.9310		3.970	.0341	.4171 1,4
N(6), H(17)	2.8623	2.8183	3.550	.0293	.1297 1,4
N(6), H(20)	2.8200	2.7798	3.550	.0293	.1617 1,4
N(6), H(23)	2.8225	2.7831	3.550	.0293	.1588 1,4
C(7), C(10)	2.8931		4.080	.0270	.5237 1,4
C(7), H(19)	2.8018	2.8115	3.560	.0230	.1108
C(7), H(23)	2.8413	2.8022	3.560	.0230	.1169 1,4
C(8), H(13)	2.8263	2.7901	3.560	.0230	.1251 1,4
C(8), H(25)	2.7967	2.7599	3.560	.0230	.1474 1,4
C(9), H(20)	2.8402	2.8011	3.560	.0230	.1176 1,4
C(10), H(13)	2.7048	2.6686	3.560	.0230	.2331 1,4
C(10), H(18)	2.6342	2.6043	3.560	.0230	.3141 1,4
C(10), H(19)	2.8335	2.7904	3.560	.0230	.1249 1,4
C(10), H(22)	2.8226	2.7841	3.560	.0230	.1293 1,4

S149

H(11), H(12)	2.5495	2.4599	3.240	.0200	.1715	1,4
H(11), H(20)	2.4668	2.3867	3.240	.0200	.2516	1,4
H(11), H(21)	2.5374	2.4489	3.240	.0200	.1821	1,4
H(11), H(23)	2.4764	2.3953	3.240	.0200	.2408	1,4
H(12), H(22)	2.4695	2.3888	3.240	.0200	.2489	1,4
H(12), H(24)	2.5240	2.4372	3.240	.0200	.1938	1,4
H(12), H(25)	2.4736	2.3919	3.240	.0200	.2450	1,4
H(13), H(14)	2.4893	2.4077	3.240	.0200	.2260	1,4
H(13), H(21)	2.4875	2.4053	3.240	.0200	.2288	1,4
H(13), H(25)	2.5088	2.5032	3.240	.0200	.1347	
H(14), H(15)	2.4418	2.3569	3.240	.0200	.2917	1,4
H(15), H(16)	2.5188	2.4353	3.240	.0200	.1957	1,4
H(16), H(18)	2.5828	2.4882	3.240	.0200	.1467	1,4
H(16), H(19)	2.4247	2.3499	3.240	.0200	.3018	1,4
H(17), H(18)	2.4125	2.3383	3.240	.0200	.3194	1,4
H(18), H(24)	2.3372	2.3466	3.240	.0200	.3067	
H(19), H(20)	2.2352	2.3002	3.240	.0200	.3830	
H(19), H(23)	2.3971	2.4473	3.240	.0200	.1836	
H(21), H(22)	2.4625	2.3822	3.240	.0200	.2573	1,4
H(23), H(24)	2.5010	2.4170	3.240	.0200	.2154	1,4

BOND ANGLES, BENDING AND STRETCH-BEND ENERGIES (51 ANGLES)

$EB = 0.021914(KB)(DT)(DT)(1+CF*DT+QF*DT**2+PF*DT**3+SF*DT**4)$
 $DT = THETA-TZERO$
 $CF = -1400.000E-5$
 $QF = 5.600E-5$
 $PF = -.070E-5$
 $SF = .022E-6$
 $ESB(J) = 2.51124(KSB(J))(DT)(DR1+DR2)$
 $DR(I) = R(I) - R0(I)$
 $EBDBD = -0.02191418(KBB1)(DT1)(KBB2)(DT2)$

A T O M S		THETA	TZERO	KB	EB	KSB	ESB	
C(2)-C(1)-N(6)	111.582	110.740	1.045	.0160	.13	.0078	C	
C(2)-C(1)-C(7)	109.610	109.800	.540	.0004	.13	-.0018		
C(2)-C(1)-H(13)	107.631	109.500	.550	.0432	.08	-.0053		
N(6)-C(1)-C(7)	111.225	108.000	.780	.1698	.13	.0386		
N(6)-C(1)-H(13)	107.855	109.300	.820	.0383	.08	-.0064		
C(7)-C(1)-H(13)	108.818	109.800	.590	.0127	.08	-.0044		
C(1)-C(2)-C(3)	123.108	122.300		.13	.0046			
IN-PLN 1- 2- 3	123.108	122.300	.470	.0067				
OUT-PL 2- 14- 2	.097	.110	.0000					
C(1)-C(2)-H(14)	117.248	117.500		.08	-.0007			
IN-PLN 1- 2- 14	117.249	117.500	.490	.0007				
OUT-PL 2- 3- 2	.079	.200	.0000					
C(3)-C(2)-H(14)	119.643	120.000		.08	-.0007			
IN-PLN 3- 2- 14	119.643	120.000	.490	.0014				
OUT-PL 2- 1- 2	.069	.100	.0000					
C(2)-C(3)-C(4)	121.911	122.300		.13	-.0016			
IN-PLN 2- 3- 4	121.919	122.300	.470	.0015				
OUT-PL 3- 15- 3	.677	.110	.0011					
C(2)-C(3)-H(15)	120.301	120.000		.08	.0006			
IN-PLN 2- 3- 15	120.312	120.000	.490	.0010				
OUT-PL 3- 4- 3	.496	.100	.0005					
C(4)-C(3)-H(15)	117.759	117.500		.08	.0004			
IN-PLN 4- 3- 15	117.769	117.500	.490	.0008				
OUT-PL 3- 2- 3	.557	.200	.0014					
C(3)-C(4)-C(5)	111.393	110.600	.540	.0074	.13	.0048		
C(3)-C(4)-H(16)	109.869	109.310	.550	.0037	.08	.0008		
C(3)-C(4)-H(17)	108.700	109.310	.550	.0045	.08	-.0010		
C(5)-C(4)-H(16)	109.684	109.310	.590	.0018	.08	.0011		
C(5)-C(4)-H(17)	110.014	109.310	.590	.0063	.08	.0021		
H(16)-C(4)-H(17)	107.080	107.600	.550	.0033				
C(4)-C(5)-N(6)	110.957	111.000	.780	.0000	.13	-.0004		
C(4)-C(5)-H(18)	108.775	109.310	.590	.0037	.08	-.0016		
C(4)-C(5)-H(19)	109.953	109.310	.590	.0053	.08	.0018		
N(6)-C(5)-H(18)	109.987	109.300	.820	.0084	.08	.0021		
N(6)-C(5)-H(19)	110.449	109.300	.820	.0233	.08	.0032		
H(18)-C(5)-H(19)	106.611	107.600	.550	.0120				

S150

C(1)- N(6)- C(5)	113.011	107.200	.720	.4905	.05	.0228
C(1)- N(6)- C(10)	112.635	107.200	.720	.4314	.05	.0220
C(5)- N(6)- C(10)	114.550	107.200	.720	.7671	.05	.0251
C(1)- C(7)- C(8)	111.882	111.000	.670	.0113	.13	.0081
C(1)- C(7)- H(20)	110.280	109.310	.590	.0120	.08	.0039
C(1)- C(7)- H(21)	109.702	109.310	.590	.0020	.08	.0017
C(8)- C(7)- H(20)	109.347	109.310	.590	.0000	.08	.0001
C(8)- C(7)- H(21)	109.286	109.310	.590	.0000	.08	-.0001
H(20)- C(7)- H(21)	106.177	107.600	.550	.0249		
C(7)- C(8)- C(9)	110.625	111.000	.670	.0021	.13	-.0022
C(7)- C(8)- H(11)	110.223	109.310	.590	.0106	.08	.0022
C(7)- C(8)- H(22)	109.435	109.310	.590	.0002	.08	.0003
C(9)- C(8)- H(11)	110.189	109.310	.590	.0099	.08	.0019
C(9)- C(8)- H(22)	109.481	109.310	.590	.0004	.08	.0004
H(11)- C(8)- H(22)	106.807	107.600	.550	.0077		
C(8)- C(9)- C(10)	110.268	111.000	.670	.0079	.13	-.0045
C(8)- C(9)- H(12)	109.980	109.310	.590	.0057	.08	.0015
C(8)- C(9)- H(23)	109.806	109.310	.590	.0032	.08	.0010
C(10)- C(9)- H(12)	110.053	109.310	.590	.0071	.08	.0020
C(10)- C(9)- H(23)	110.071	109.310	.590	.0074	.08	.0019
H(12)- C(9)- H(23)	106.596	107.600	.550	.0123		
N(6)- C(10)- C(9)	113.158	111.000	.780	.0772	.13	.0174
N(6)- C(10)- H(24)	109.840	109.300	.820	.0052	.08	.0017
N(6)- C(10)- H(25)	108.707	109.300	.820	.0064	.08	-.0020
C(9)- C(10)- H(24)	110.090	109.310	.590	.0078	.08	.0019
C(9)- C(10)- H(25)	108.965	109.310	.590	.0015	.08	-.0009
H(24)- C(10)- H(25)	105.802	107.600	.550	.0399		

DIHEDRAL ANGLES, TORSIONAL ENERGY (ET) (79 ANGLES)

$$ET = (V1/2)(1+\cos(W)) + (V2/2)(1-\cos(2W)) + (V3/2)(1+\cos(3W))$$

$$ETS = -11.995 \cdot (R-R0) \cdot ((KTS1/2)(1+\cos(W)) + (KTS2/2)(1-\cos(2W)) + (KTS3/2)(1+\cos(3W)))$$

SIGN OF ANGLE A-B-C-D : WHEN LOOKING THROUGH B TOWARD C,
IF D IS COUNTERCLOCKWISE FROM A, NEGATIVE.

A T O M S				OMEGA	V1	V2	V3	ET	KTS3	ETS
C(1) C(2) C(3) C(4)	-9	-300	9.500	.000	-.298					
C(1) C(2) C(3) H(15)	-178.9	.000	10.000	.000	.004					
C(1) N(6) C(5) C(4)	62.5	.958	-.155	.766	.582	.061	.000			
C(1) N(6) C(5) H(18)	-177.1	.072	-.012	.563	.003	.061	.000			
C(1) N(6) C(5) H(19)	-59.7	.072	-.012	.563	.045	.061	.000			
C(1) N(6) C(10) C(9)	56.8	.958	-.155	.766	.639	.061	.000			
C(1) N(6) C(10) H(24)	-179.8	.072	-.012	.563	.000	.061	.000			
C(1) N(6) C(10) H(25)	-64.4	.072	-.012	.563	.049	.061	.000			
C(1) C(7) C(8) C(9)	-52.8	.185	.170	.520	.275	.059	.000			
C(1) C(7) C(8) H(11)	-174.9	.000	.000	.280	.005	.059	.000			
C(1) C(7) C(8) H(22)	67.9	.000	.000	.280	.012	.059	.000			
C(2) C(1) N(6) C(5)	-46.1	.000	.000	.000	.000	.061	-.002	C		
C(2) C(1) N(6) C(10)	-177.9	.000	.000	.000	.000	.061	.000	C		
C(2) C(1) C(7) C(8)	177.6	.200	-.200	1.300	.005	.059	.000			
C(2) C(1) C(7) H(20)	55.7	.000	.000	.500	.006	.059	.000			
C(2) C(1) C(7) H(21)	-60.9	.000	.000	.500	.000	.059	.000			
C(2) C(3) C(4) C(5)	15.4	-.700	-.200	-.550	-1.166					
C(2) C(3) C(4) H(16)	137.2	.000	.000	-.090	-.073					
C(2) C(3) C(4) H(17)	-105.9	.000	.000	-.090	-.078					
C(3) C(2) C(1) N(6)	15.4	.000	.000	.000	.000			C		
C(3) C(2) C(1) C(7)	-108.3	-.700	-.200	-.550	-.920					
C(3) C(2) C(1) H(13)	133.5	.000	.000	-.090	-.079					
C(3) C(4) C(5) N(6)	-44.8	.000	.000	.180	.027	.059	-.001	C		
C(3) C(4) C(5) H(18)	-166.0	.000	.000	.500	.065	.059	-.001			
C(3) C(4) C(5) H(19)	77.6	.000	.000	.500	.099	.059	-.002			
C(4) C(3) C(2) H(14)	179.4	.000	10.000	.000	.001					
C(4) C(5) N(6) C(10)	-166.7	.958	-.155	.766	.094	.061	-.001			
C(5) C(4) C(3) H(15)	-166.5	.000	.000	.010	.001	.270	-.002			
C(5) N(6) C(1) C(7)	76.6	.958	-.155	.766	.579	.061	-.002			
C(5) N(6) C(1) H(13)	-164.1	.072	-.012	.563	.092	.061	-.002			

S151

```

C( 5) N( 6) C( 10) C( 9) -74.3 .958 -.155 .766 .567 .061 -.001
C( 5) N( 6) C( 10) H( 24) 49.2 .072 -.012 .563 .096 .061 -.001
C( 5) N( 6) C( 10) H( 25) 164.5 .072 -.012 .563 .088 .061 -.002
N( 6) C( 1) C( 2) H( 14) -164.9 .000 .000 .000 .000 .270 -.005 C
N( 6) C( 1) C( 7) C( 8) 53.7 -.302 .696 .499 .225 .059 .000
N( 6) C( 1) C( 7) H( 20) -68.2 .000 .000 .374 .017 .059 -.001
N( 6) C( 1) C( 7) H( 21) 175.2 .000 .000 .374 .006 .059 .000
N( 6) C( 5) C( 4) H( 16) -166.7 .000 .000 .374 .044 .059 -.001
N( 6) C( 5) C( 4) H( 17) 75.8 .000 .000 .374 .060 .059 -.001
N( 6) C( 10) C( 9) C( 8) -54.8 -.302 .696 .499 .236 .059 .000
N( 6) C( 10) C( 9) H( 12) -176.3 .000 .000 .374 .003 .059 .000
N( 6) C( 10) C( 9) H( 23) 66.5 .000 .000 .374 .011 .059 .000
C( 7) C( 1) C( 2) H( 14) 71.4 .000 .000 .010 .001 .270 -.003
C( 7) C( 1) N( 6) C( 10) -55.2 .958 -.155 .766 .660 .061 .000
C( 7) C( 8) C( 9) C( 10) 52.4 .185 .170 .520 .276 .059 .000
C( 7) C( 8) C( 9) H( 12) 173.9 .000 .000 .280 .007 .059 .000
C( 7) C( 8) C( 9) H( 23) -69.1 .000 .000 .280 .015 .059 .000
C( 8) C( 7) C( 1) H( 13) -64.9 .000 .000 .280 .005 .059 .000
C( 8) C( 9) C( 10) H( 24) -178.1 .000 .000 .280 .001 .059 .000
C( 8) C( 9) C( 10) H( 25) 66.3 .000 .000 .280 .007 .059 .000
C( 9) C( 8) C( 7) H( 20) 69.7 .000 .000 .280 .018 .059 .000
C( 9) C( 8) C( 7) H( 21) -174.5 .000 .000 .280 .006 .059 .000
C( 10) N( 6) C( 1) H( 13) 64.1 .072 -.012 .563 .048 .061 .000
C( 10) N( 6) C( 5) H( 18) -46.3 .072 -.012 .563 .124 .061 -.001
C( 10) N( 6) C( 5) H( 19) 71.1 .072 -.012 .563 .083 .061 -.001
C( 10) C( 9) C( 8) H( 11) 174.5 .000 .000 .280 .006 .059 .000
C( 10) C( 9) C( 8) H( 22) -68.3 .000 .000 .280 .013 .059 .000
H( 11) C( 8) C( 7) H( 20) -52.4 .000 .000 .238 .009 .059 .000
H( 11) C( 8) C( 7) H( 21) 63.4 .000 .000 .238 .002 .059 .000
H( 11) C( 8) C( 9) H( 12) -63.9 .000 .000 .238 .002 .059 .000
H( 11) C( 8) C( 9) H( 23) 53.1 .000 .000 .238 .008 .059 .000
H( 12) C( 9) C( 8) H( 22) 53.3 .000 .000 .238 .007 .059 .000
H( 12) C( 9) C( 10) H( 24) 60.4 .000 .000 .238 .000 .059 .000
H( 12) C( 9) C( 10) H( 25) -55.2 .000 .000 .238 .004 .059 .000
H( 13) C( 1) C( 2) H( 14) -46.8 .000 .000 .580 .067 .270 -.004
H( 13) C( 1) C( 7) H( 20) 173.1 .000 .000 .238 .008 .059 .000
H( 13) C( 1) C( 7) H( 21) 56.5 .000 .000 .238 .002 .059 .000
H( 14) C( 2) C( 3) H( 15) 1.4 .000 11.500 .000 .007
H( 15) C( 3) C( 4) H( 16) -44.8 .000 .000 .580 .087 .270 -.003
H( 15) C( 3) C( 4) H( 17) 72.1 .000 .000 .580 .056 .270 -.002
H( 16) C( 4) C( 5) H( 18) 72.2 .000 .000 .238 .023 .059 -.001
H( 16) C( 4) C( 5) H( 19) -44.2 .000 .000 .238 .038 .059 -.001
H( 17) C( 4) C( 5) H( 18) -45.3 .000 .000 .238 .033 .059 -.001
H( 17) C( 4) C( 5) H( 19) -161.7 .000 .000 .238 .050 .059 -.002
H( 20) C( 7) C( 8) H( 22) -169.6 .000 .000 .238 .017 .059 .000
H( 21) C( 7) C( 8) H( 22) -53.8 .000 .000 .238 .006 .059 .000
H( 22) C( 8) C( 9) H( 23) 170.3 .000 .000 .238 .015 .059 .000
H( 23) C( 9) C( 10) H( 24) -56.8 .000 .000 .238 .002 .059 .000
H( 23) C( 9) C( 10) H( 25) -172.4 .000 .000 .238 .009 .059 .000

```

DIPOLE-DIPOLE INTERACTION ENERGY (DIELECTRIC CONSTANT = 1.50)

$$E = 14.388 * MU1 * MU2 * (COSX - 3 * COSA * COSB) / (R12 ** 3 * DIELC)$$

MU1 = BOND MOM OF BOND 1

MU2 = BOND MOM OF BOND 2

R12 = DISTANCE BETWEEN MID-POINTS OF TWO BONDS.

(ENERGIES LESS THAN 0.2 KCAL/MOL ARE NOT PRINTED.)

BOND(1)	MU1	BOND(2)	MU2	R12	E
C(1)- C(2)	.900	+ C(3)- C(4)	-.900	2.1489	1.0090
C(1)- C(2)	.900	+ C(3)- H(15)	-.600	2.3125	.5298
C(1)- C(2)	.900	+ C(5)- N(6)	.680	2.0997	-.6869
C(1)- C(2)	.900	+ N(6)- C(10)	-.680	2.4484	-.4307
C(1)- N(6)	.680	+ C(2)- H(14)	-.600	2.3406	-.2991
C(1)- N(6)	.680	+ C(3)- C(4)	-.900	2.4801	-.3700
C(2)- H(14)	-.600	+ C(3)- C(4)	-.900	2.2998	.5296
C(2)- H(14)	-.600	+ C(3)- H(15)	-.600	1.8904	.6387
C(3)- C(4)	-.900	+ C(5)- N(6)	.680	2.1349	.6400

 NORMAL MODE VIBRATIONAL ANALYSIS

Molecular Shape : ASYMMETRIC ROTOR WITH KAPPA = -.698012
 Symmetry Point Group : C1
 Symmetry Number : 1
 Chirality : yes

0 FUNDAMENTAL NORMAL VIBRATIONAL FREQUENCIES
 (THEORETICALLY 69 VALUES)

Frequency : in 1/cm
 A(i) : IR intensity (vs,s,m,w,vw,-- or in 10**6 cm/mole)
 A(i) = -- : IR inactive

no	Frequency	Symmetry	A(i)
1.	3051.0	(A)	m
2.	3036.6	(A)	w
3.	2940.9	(A)	m
4.	2935.2	(A)	s
5.	2934.9	(A)	m
6.	2933.7	(A)	m
7.	2931.1	(A)	w
8.	2926.7	(A)	m
9.	2917.4	(A)	m
10.	2893.9	(A)	m
11.	2885.9	(A)	m
12.	2883.4	(A)	m
13.	2880.3	(A)	m
14.	2869.3	(A)	m
15.	2797.9	(A)	m
16.	1691.3	(A)	w
17.	1591.3	(A)	w
18.	1566.9	(A)	w
19.	1553.4	(A)	w
20.	1517.7	(A)	w
21.	1480.4	(A)	w
22.	1475.6	(A)	w
23.	1468.3	(A)	w
24.	1466.6	(A)	w
25.	1451.2	(A)	w
26.	1436.3	(A)	w
27.	1410.9	(A)	w
28.	1405.6	(A)	w
29.	1391.3	(A)	w
30.	1382.1	(A)	w
31.	1359.9	(A)	m
32.	1320.3	(A)	w
33.	1317.5	(A)	w
34.	1252.1	(A)	w
35.	1228.8	(A)	vw
36.	1214.6	(A)	w
37.	1208.3	(A)	w
38.	1198.5	(A)	w
39.	1174.8	(A)	w
40.	1155.6	(A)	w
41.	1095.0	(A)	w
42.	1075.3	(A)	vw
43.	1053.9	(A)	w
44.	1034.7	(A)	w
45.	1013.4	(A)	w
46.	980.8	(A)	w
47.	972.8	(A)	w
48.	937.1	(A)	w

49.	928.3	(A)	w
50.	907.9	(A)	w
51.	860.0	(A)	w
52.	843.8	(A)	w
53.	833.2	(A)	w
54.	817.3	(A)	w
55.	766.3	(A)	w
56.	674.8	(A)	w
57.	663.1	(A)	m
58.	582.2	(A)	w
59.	508.7	(A)	w
60.	479.4	(A)	w
61.	439.6	(A)	w
62.	409.3	(A)	w
63.	381.0	(A)	w
64.	365.9	(A)	w
65.	301.8	(A)	w
66.	276.0	(A)	w
67.	202.2	(A)	w
68.	173.5	(A)	vw
69.	121.1	(A)	w
70.	(.0)	(t/r)	
71.	(.0)	(t/r)	
72.	(.0)	(t/r)	
73.	(.0)	(t/r)	
74.	(.0)	(t/r)	
75.	(.0)	(t/r)	

=====

STATISTICAL THERMODYNAMICS ANALYSIS

=====

Structure name : RINI
 Temperature : 298.16 K
 Symmetry number : 1
 Optical isomers : 2
 Zero Point Energy : 140.433 Kcal/mol

	ENERGY (Kcal/mol)	ENTHALPY (Kcal/mol)	ENTROPY (eu)	FREE ENERGY (Kcal/mol)	HEAT CAPACITY (cal/mol/deg)
Translational	.889	1.481	40.641	-10.636	4.967
Rotational	.889	.889	29.190	-7.815	2.980
Vibrational	144.083%	144.083%	19.434*	138.288%	30.200*
Potential	17.870#	17.870#	.000	17.870#	.000
Mixing	.000	.000	1.377	-.411	.000
Total	163.730	164.322	90.641	137.297	38.148

Enthalpy Function (H-Ho)/T = 20.19 cal/mol/deg
 Free Energy Function -(G-Ho)/T = 70.45 cal/mol/deg

% Includes zero point energy (ZPE).
 * Excludes contribution from frequencies lower than 40 (1/cm).
 # Includes steric energy (SE).
 Internal rotation contributions are not considered

This structure has 0 imaginary frequencies,
 0 free internal rotation (fir) frequencies
 (>= 0, < 10 /cm),
 0 restricted internal rotation (rir) frequencies
 (>= 10, < 40 /cm),
 6 zero frequencies, and
 69 real frequencies.

FINAL STERIC ENERGY IS 17.8698 KCAL/MOL.

COMPRESSION .6155
 BENDING 2.3269

BEND-BEND -.1399
 STRETCH-BEND .1502
 VANDERWAALS
 1,4 ENERGY 10.4699
 OTHER -.2671

TORSIONAL 3.0459
 TORSION-STRETCH -.0517
 DIPOLE-DIPOLE 1.7199
 CHARGE-DIPOLE .0000
 CHARGE-CHARGE .0000

COORDINATES TRANSLATED TO NEW ORIGIN WHICH IS CENTER OF MASS

C(1)	-.07481	-.79329	.59200	(1)
C(2)	-1.48072	-1.30125	.38426	(2)
C(3)	-2.47553	-.53251	-.07666	(2)
C(4)	-2.26951	.92046	-.40844	(1)
C(5)	-.77936	1.26288	-.51932	(1)
N(6)	-.02395	.67195	.58294	(8)
C(7)	.85655	-1.39153	-.48414	(1)
C(8)	2.28920	-.86283	-.35744	(1)
C(9)	2.29912	.66802	-.33496	(1)
C(10)	1.33544	1.18875	.73360	(1)
H(11)	2.91456	-1.23915	-1.19952	(5)
H(12)	3.33002	1.03909	-.13314	(5)
H(13)	.26506	-1.14094	1.59531	(5)
H(14)	-1.67612	-2.36050	.62528	(5)
H(15)	-3.49141	-.94725	-.19320	(5)
H(16)	-2.78316	1.16669	-1.36528	(5)
H(17)	-2.74469	1.53915	.38656	(5)
H(18)	-.66441	2.37022	-.50890	(5)
H(19)	-.37650	.90726	-1.50663	(5)
H(20)	.46752	-1.16242	-1.50177	(5)
H(21)	.86524	-2.50262	-.39794	(5)
H(22)	2.74617	-1.25135	.58204	(5)
H(23)	2.00949	1.06193	-1.33534	(5)
H(24)	1.31966	2.30134	.72456	(5)
H(25)	1.71822	.89916	1.73803	(5)

MOMENT OF INERTIA WITH THE PRINCIPAL AXES

(1) UNIT = 10**(-39) GM*CM**2
 IX= 33.8770 IY= 72.9273 IZ= 91.7332

(2) UNIT = AU A**2
 IX= 204.0345 IY= 439.2264 IZ= 552.4909

DIPOLE MOMENT = .745 D

COMPONENTS WITH PRINCIPAL AXES

X = -.5601 Y = -.2065 Z = .4457

Compound 8 (conformer 2)CONFORMATIONAL ENERGY, PART 3: GEOMETRY AND STERIC ENERGY
OF FINAL CONFORMATION.

CONNECTED ATOMS

1- 2- 3- 4- 5- 6- 10- 9-

1- 6-

1- 7- 8- 9-

ATTACHED ATOMS

8- 11, 9- 12, 1- 13, 2- 14, 3- 15, 4- 16, 4- 17,

5- 18, 5- 19, 7- 20, 7- 21, 8- 22, 9- 23, 10- 24,

10- 25,

FINAL ATOMIC COORDINATE

ATOM	X	Y	Z	TYPE
C(1)	.00785	.69180	.42586	(1)
C(2)	1.30493	1.42458	.17893	(2)
C(3)	2.43701	.79929	-.16762	(2)
C(4)	2.49380	-.69509	-.33017	(1)
C(5)	1.25411	-1.36170	.27698	(1)
N(6)	.03738	-.66431	-.13287	(8)
C(7)	-1.17176	1.44547	-.21111	(1)
C(8)	-2.49835	.72848	.06565	(1)
C(9)	-2.41875	-.73932	-.36357	(1)
C(10)	-1.17127	-1.41065	.21628	(1)
H(11)	-3.33208	1.24060	-.46767	(5)
H(12)	-3.33497	-1.28412	-.04006	(5)
H(13)	-.14563	.64006	1.54175	(5)
H(14)	1.30209	2.52159	.29806	(5)
H(15)	3.35837	1.37521	-.35943	(5)
H(16)	2.56571	-.93644	-1.41508	(5)
H(17)	3.41198	-1.09463	.15692	(5)
H(18)	1.33086	-1.37562	1.40046	(5)
H(19)	1.21841	-2.42310	-.05767	(5)
H(20)	-1.01483	1.52943	-1.31116	(5)
H(21)	-1.22406	2.48461	.18767	(5)
H(22)	-2.72988	.78455	1.15456	(5)
H(23)	-2.38529	-.79717	-1.47606	(5)
H(24)	-1.10275	-2.44615	-.18705	(5)
H(25)	-1.26527	-1.50036	1.33460	(5)

DIELECTRIC CONSTANT = 1.500

BOND LENGTHS AND STRETCHING ENERGY (26 BONDS)

ENERGY = 71.94(KS)(DR)(DR)(1-(CS)(DR)+(7/12)((CS)(DR))**2)

DR = R-RO

CS = 2.550

BOND	LENGTH	R(0)	K(S)	R(0)-CORR ENERGY	CORR E-NEG	MISCEL	KS
C(1)- C(2)	1.5101	1.4990	6.300	.0542			
C(1)- N(6)	1.4670	1.4480	5.300	.1312			
C(1)- C(7)	1.5379	1.5225	4.490	.0736	-.0050	.0028	HY
C(1)- H(13)	1.1276	1.1232	4.443	.0059	-.0011	.0123	BH -.367
C(2)- C(3)	1.3389	1.3320	7.500	.0253			
C(2)- H(14)	1.1035	1.1010	5.150	.0022			
C(3)- C(4)	1.5043	1.4990	6.300	.0124			
C(3)- H(15)	1.1033	1.1010	5.150	.0020			
C(4)- C(5)	1.5329	1.5201	4.490	.0516	-.0050	.0004	HY
C(4)- H(16)	1.1138	1.1116	4.694	.0016	-.0004		.014
C(4)- H(17)	1.1135	1.1116	4.694	.0013	-.0004		.014
C(5)- N(6)	1.4611	1.4480	5.300	.0631			
C(5)- H(18)	1.1262	1.1233	4.310	.0025	-.0011	.0124	BH -.370
C(5)- H(19)	1.1135	1.1113	4.701	.0015	-.0011	.0004	BH .021
N(6)- C(10)	1.4628	1.4480	5.300	.0804			
C(7)- C(8)	1.5331	1.5227	4.490	.0343	-.0020		
C(7)- H(20)	1.1144	1.1116	4.694	.0026	-.0004		.014

S156

```

C( 7)- H( 21) 1.1143 1.1116 4.694 .0024 -.0004 .014
C( 8)- C( 9) 1.5313 1.5227 4.490 .0236 -.0020
C( 8)- H( 11) 1.1144 1.1120 4.680 .0019
C( 8)- H( 22) 1.1147 1.1120 4.680 .0024
C( 9)- C( 10) 1.5307 1.5197 4.490 .0381 -.0050
C( 9)- H( 12) 1.1140 1.1116 4.694 .0019 -.0004 .014
C( 9)- H( 23) 1.1145 1.1116 4.694 .0029 -.0004 .014
C( 10)- H( 24) 1.1134 1.1111 4.708 .0017 -.0011 .0002 BH .028
C( 10)- H( 25) 1.1258 1.1235 4.305 .0017 -.0011 .0126 BH -.375

```

NON-BONDED DISTANCES, VDW AND EPR ENERGY (223 PAIRS)

```

E(VDW) = KV*(1.84(10**5)EXP(-12.00/P) - 2.25(P**6))
E(EPR) = C*KV*(1.84(10**5)EXP(-12.00/Q) - 2.25(Q**6))
E(HBD) = EP1-EP2*COS(THETA)*RTH/RTH0
          EP1 = KHB*1.84(10**5)*EXP(-12.0/P)
          EP2 = KHB*2.25(P**6)

```

IF P > 3.020, THEN,

```

E(VDW) = KV(192.270)(P**2)
E(HBD) = EP1-EP2*COS(THETA)*RTH/RTH0
          EP1 = KHB*(192.270*P**2+1706.96)
          EP2 = KHB*1706.96

```

WHERE RV = RVDW(I) + RVDW(K)

KV = SQRT(EPS(I)*EPS(K))

KHB = EPS/DIELEC FOR HYDROGEN BOND

P = (RV/R) OR (RV/R#)

C = SCALE FACTOR

Q = RV/R, WHERE R IS MODIFIED DISTANCE

THETA = ANGLE H-X-Y IN HYDROGEN BOND X-H...Y

RTH = BOND LENGTH X-H IN X-H...Y

RTH0 = NATURAL BOND LENGTH X-H

IN THE VDW CALCULATIONS THE HYDROGEN ATOMS ARE RELOCATED
SO THAT THE ATTACHED HYDROGEN DISTANCE IS REDUCED BY .923

IN THE VDW CALCULATIONS THE DEUTERIUM ATOMS ARE RELOCATED
SO THAT THE ATTACHED DEUTERIUM DISTANCE IS REDUCED BY .923

** INTERACTIONS OF LESS THAN 0.1 KCAL/MOL ARE NOT PRINTED **

ATOM PAIR	R	R#	RV	KV	ENERGY
C(1), C(4)	2.9453		4.080	.0270	.4298 1,4
C(1), C(9)	2.9257		4.080	.0270	.4633 1,4
C(1), H(18)	2.6409	2.6064	3.560	.0230	.3111 1,4
C(1), H(22)	2.8346	2.7967	3.560	.0230	.1206 1,4
C(1), H(25)	2.6930	2.6560	3.560	.0230	.2474 1,4
C(2), C(5)	2.7885		4.000	.0389	.9032 1,4
C(2), H(20)	2.7591	2.7244	3.580	.0335	.2783 1,4
C(2), H(21)	2.7422	2.7086	3.580	.0335	.3007 1,4
C(3), N(6)	2.8110		3.890	.0491	.7723 1,4
C(3), H(18)	2.9005	2.8561	3.580	.0335	.1362 1,4
C(5), H(13)	2.7506	2.7091	3.560	.0230	.1913 1,4
C(5), H(24)	2.6356	2.6032	3.560	.0230	.3157 1,4
C(5), H(25)	2.7359	2.6967	3.560	.0230	.2034 1,4
N(6), C(8)	2.8999		3.970	.0341	.4736 1,4
N(6), H(16)	2.8479	2.8046	3.550	.0293	.1406 1,4
N(6), H(20)	2.7033	2.6670	3.550	.0293	.2889 1,4
N(6), H(23)	2.7733	2.7349	3.550	.0293	.2057 1,4
C(7), C(10)	2.8879		4.080	.0270	.5340 1,4
C(7), H(14)	2.7454	2.7119	3.560	.0230	.1886 1,4
C(7), H(23)	2.8464	2.8070	3.560	.0230	.1138 1,4
C(8), H(13)	2.7788	2.7442	3.560	.0230	.1600 1,4
C(8), H(25)	2.8458	2.8062	3.560	.0230	.1143 1,4
C(9), H(20)	2.8313	2.7928	3.560	.0230	.1232 1,4
C(10), H(13)	2.6484	2.6143	3.560	.0230	.3002 1,4
C(10), H(18)	2.7684	2.7271	3.560	.0230	.1747 1,4
C(10), H(19)	2.6097	2.5791	3.560	.0230	.3516 1,4
C(10), H(22)	2.8510	2.8114	3.560	.0230	.1109 1,4

H(11), H(12)	2.5607	2.4700	3.240	.0200	.1624	1,4
H(11), H(20)	2.4829	2.4011	3.240	.0200	.2338	1,4
H(11), H(21)	2.5339	2.4459	3.240	.0200	.1850	1,4
H(11), H(23)	2.4629	2.3830	3.240	.0200	.2562	1,4
H(12), H(22)	2.4643	2.3843	3.240	.0200	.2545	1,4
H(12), H(24)	2.5209	2.4336	3.240	.0200	.1976	1,4
H(12), H(25)	2.4940	2.4112	3.240	.0200	.2220	1,4
H(13), H(18)	2.5026	2.4946	3.240	.0200	.1415	
H(13), H(21)	2.5296	2.4426	3.240	.0200	.1883	1,4
H(13), H(25)	2.4244	2.4240	3.240	.0200	.2077	
H(14), H(15)	2.4443	2.3592	3.240	.0200	.2884	1,4
H(14), H(21)	2.5288	2.5260	3.240	.0200	.1179	
H(15), H(17)	2.5238	2.4399	3.240	.0200	.1911	1,4
H(16), H(19)	2.4224	2.3470	3.240	.0200	.3061	1,4
H(17), H(18)	2.4406	2.3641	3.240	.0200	.2815	1,4
H(17), H(19)	2.5734	2.4799	3.240	.0200	.1537	1,4
H(19), H(24)	2.3249	2.3326	3.240	.0200	.3282	
H(21), H(22)	2.4683	2.3874	3.240	.0200	.2506	1,4
H(23), H(24)	2.4547	2.3745	3.240	.0200	.2673	1,4

BOND ANGLES, BENDING AND STRETCH-BEND ENERGIES (51 ANGLES)

$$EB = 0.021914(KB)(DT)(DT)(1+CF*DT+QF*DT**2+PF*DT**3+SF*DT**4)$$

$$DT = THETA-TZERO$$

$$CF = -1400.000E-5$$

$$QF = 5.600E-5$$

$$PF = -.070E-5$$

$$SF = .022E-6$$

$$ESB(J) = 2.51124(KSB(J))(DT)(DR1+DR2)$$

$$DR(I) = R(I) - R0(I)$$

$$EBDBD = -0.02191418(KBB1)(DT1)(KBB2)(DT2)$$

A T O M S						THETA	TZERO	KB	EB	KSB	ESB	
C(2)-C(1)-N(6)	111.654	110.740	1.045	.0189	.13	.0090						C
C(2)-C(1)-C(7)	110.689	109.800	.540	.0092	.13	.0077						
C(2)-C(1)-H(13)	107.518	109.500	.550	.0487	.08	-.0061						
N(6)-C(1)-C(7)	108.102	108.000	.780	.0002	.13	.0011						
N(6)-C(1)-H(13)	109.709	109.300	.820	.0030	.08	.0019						
C(7)-C(1)-H(13)	109.145	109.800	.590	.0056	.08	-.0026						
C(1)-C(2)-C(3)	122.817	122.300		.13	.0030							
IN-PLN	1-	2-	3	122.817	122.300	.470	.0027					
OUT-PL	2-	14-	2	.093	.110	.0000						
C(1)-C(2)-H(14)	117.552	117.500		.08	.0001							
IN-PLN	1-	2-	14	117.552	117.500	.490	.0000					
OUT-PL	2-	3-	2	.074	.200	.0000						
C(3)-C(2)-H(14)	119.630	120.000		.08	-.0007							
IN-PLN	3-	2-	14	119.630	120.000	.490	.0015					
OUT-PL	2-	1-	2	.066	.100	.0000						
C(2)-C(3)-C(4)	121.590	122.300		.13	-.0028							
IN-PLN	2-	3-	4	121.592	122.300	.470	.0052					
OUT-PL	3-	15-	3	.336	.110	.0003						
C(2)-C(3)-H(15)	120.483	120.000		.08	.0009							
IN-PLN	2-	3-	15	120.486	120.000	.490	.0025					
OUT-PL	3-	4-	3	.246	.100	.0001						
C(4)-C(3)-H(15)	117.920	117.500		.08	.0006							
IN-PLN	4-	3-	15	117.922	117.500	.490	.0019					
OUT-PL	3-	2-	3	.277	.200	.0003						
C(3)-C(4)-C(5)	111.019	110.600	.540	.0021	.13	.0025						
C(3)-C(4)-H(16)	108.843	109.310	.550	.0026	.08	-.0007						
C(3)-C(4)-H(17)	109.896	109.310	.550	.0041	.08	.0009						
C(5)-C(4)-H(16)	110.108	109.310	.590	.0082	.08	.0024						
C(5)-C(4)-H(17)	109.728	109.310	.590	.0022	.08	.0012						
H(16)-C(4)-H(17)	107.164	107.600	.550	.0023								
C(4)-C(5)-N(6)	110.781	111.000	.780	.0008	.13	-.0019						
C(4)-C(5)-H(18)	110.205	109.310	.590	.0102	.08	.0028						
C(4)-C(5)-H(19)	108.748	109.310	.590	.0041	.08	-.0017						
N(6)-C(5)-H(18)	110.029	109.300	.820	.0095	.08	.0023						
N(6)-C(5)-H(19)	110.120	109.300	.820	.0119	.08	.0025						
H(18)-C(5)-H(19)	106.872	107.600	.550	.0065								
C(1)-N(6)-C(5)	110.558	107.200	.720	.1697	.05	.0135						

S158

```

C( 1)-N( 6)-C( 10) 111.352 107.200 .720 .2564 .05 .0176
C( 5)-N( 6)-C( 10) 112.185 107.200 .720 .3652 .05 .0174
C( 1)-C( 7)-C( 8) 111.084 111.000 .670 .0001 .13 .0007
C( 1)-C( 7)-H( 20) 109.741 109.310 .590 .0024 .08 .0016
C( 1)-C( 7)-H( 21) 110.169 109.310 .590 .0094 .08 .0031
C( 8)-C( 7)-H( 20) 109.591 109.310 .590 .0010 .08 .0007
C( 8)-C( 7)-H( 21) 109.324 109.310 .590 .0000 .08 .0000
H( 20)-C( 7)-H( 21) 106.836 107.600 .550 .0071
C( 7)-C( 8)-C( 9) 110.651 111.000 .670 .0018 .13 -.0022
C( 7)-C( 8)-H( 11) 110.247 109.310 .590 .0112 .08 .0024
C( 7)-C( 8)-H( 22) 109.424 109.310 .590 .0002 .08 .0003
C( 9)-C( 8)-H( 11) 110.196 109.310 .590 .0100 .08 .0020
C( 9)-C( 8)-H( 22) 109.440 109.310 .590 .0002 .08 .0003
H( 11)-C( 8)-H( 22) 106.799 107.600 .550 .0078
C( 8)-C( 9)-C( 10) 110.889 111.000 .670 .0002 .13 -.0007
C( 8)-C( 9)-H( 12) 110.158 109.310 .590 .0092 .08 .0019
C( 8)-C( 9)-H( 23) 109.336 109.310 .590 .0000 .08 .0001
C( 10)-C( 9)-H( 12) 110.230 109.310 .590 .0108 .08 .0025
C( 10)-C( 9)-H( 23) 109.324 109.310 .590 .0000 .08 .0000
H( 12)-C( 9)-H( 23) 106.810 107.600 .550 .0076
N( 6)-C( 10)-C( 9) 111.050 111.000 .780 .0000 .13 .0004
N( 6)-C( 10)-H( 24) 109.707 109.300 .820 .0030 .08 .0014
N( 6)-C( 10)-H( 25) 110.288 109.300 .820 .0173 .08 .0034
C( 9)-C( 10)-H( 24) 108.712 109.310 .590 .0047 .08 -.0016
C( 9)-C( 10)-H( 25) 110.071 109.310 .590 .0074 .08 .0020
H( 24)-C( 10)-H( 25) 106.909 107.600 .550 .0058

```

DIHEDRAL ANGLES, TORSIONAL ENERGY (ET) (79 ANGLES)

$$ET = (V1/2)(1+\cos(W)) + (V2/2)(1-\cos(2W)) + (V3/2)(1+\cos(3W))$$

$$ETS = -11.995 \cdot (R-R0) \cdot ((KTS1/2)(1+\cos(W)) + (KTS2/2)(1-\cos(2W)) + (KTS3/2)(1+\cos(3W)))$$

SIGN OF ANGLE A-B-C-D : WHEN LOOKING THROUGH B TOWARD C,
IF D IS COUNTERCLOCKWISE FROM A, NEGATIVE.

ATOMS	OMEGA	V1	V2	V3	ET	KTS3	ETS
C(1) C(2) C(3) C(4)	-3	-.300	9.500	.000	-.300		
C(1) C(2) C(3) H(15)	178.7	.000	10.000	.000	.005		
C(1) N(6) C(5) C(4)	-65.8	.958	-.155	.766	.564	.061	.000
C(1) N(6) C(5) H(18)	56.4	.072	-.012	.563	.053	.061	.000
C(1) N(6) C(5) H(19)	173.9	.072	-.012	.563	.014	.061	.000
C(1) N(6) C(10) C(9)	62.0	.958	-.155	.766	.585	.061	.000
C(1) N(6) C(10) H(24)	-177.8	.072	-.012	.563	.002	.061	.000
C(1) N(6) C(10) H(25)	-60.3	.072	-.012	.563	.045	.061	.000
C(1) C(7) C(8) C(9)	-53.4	.185	.170	.520	.273	.059	.000
C(1) C(7) C(8) H(11)	-175.6	.000	.000	.280	.004	.059	.000
C(1) C(7) C(8) H(22)	67.3	.000	.000	.280	.010	.059	.000
C(2) C(1) N(6) C(5)	49.3	.000	.000	.000	.000	.061	-.001 C
C(2) C(1) N(6) C(10)	174.7	.000	.000	.000	.000	.061	.000 C
C(2) C(1) C(7) C(8)	-178.5	.200	-.200	1.300	.002	.059	.000
C(2) C(1) C(7) H(20)	60.1	.000	.000	.500	.000	.059	.000
C(2) C(1) C(7) H(21)	-57.2	.000	.000	.500	.003	.059	.000
C(2) C(3) C(4) C(5)	-14.1	-.700	-.200	-.550	-1.179		
C(2) C(3) C(4) H(16)	107.2	.000	.000	-.090	-.080		
C(2) C(3) C(4) H(17)	-135.7	.000	.000	-.090	-.076		
C(3) C(2) C(1) N(6)	-16.9	.000	.000	.000	.000		C
C(3) C(2) C(1) C(7)	-137.4	-.700	-.200	-.550	-.628		
C(3) C(2) C(1) H(13)	103.5	.000	.000	-.090	-.074		
C(3) C(4) C(5) N(6)	46.3	.000	.000	.180	.022	.059	-.001 C
C(3) C(4) C(5) H(18)	-75.7	.000	.000	.500	.080	.059	-.001
C(3) C(4) C(5) H(19)	167.5	.000	.000	.500	.052	.059	-.001
C(4) C(3) C(2) H(14)	179.4	.000	10.000	.000	.001		
C(4) C(5) N(6) C(10)	169.3	.958	-.155	.766	.062	.061	-.001
C(5) C(4) C(3) H(15)	166.9	.000	.000	.010	.001	.270	-.002
C(5) N(6) C(1) C(7)	171.3	.958	-.155	.766	.041	.061	-.001
C(5) N(6) C(1) H(13)	-69.8	.072	-.012	.563	.074	.061	-.001
C(5) N(6) C(10) C(9)	-173.5	.958	-.155	.766	.023	.061	.000

S159

```

C( 5) N( 6) C( 10) H( 24) -53.3 .072 -.012 .563 .067 .061 .000
C( 5) N( 6) C( 10) H( 25) 64.2 .072 -.012 .563 .049 .061 .000
N( 6) C( 1) C( 2) H( 14) 163.4 .000 .000 .000 .000 .270 -.006 C
N( 6) C( 1) C( 7) C( 8) 58.9 -.302 .696 .499 .282 .059 .000
N( 6) C( 1) C( 7) H( 20) -62.4 .000 .000 .374 .002 .059 .000
N( 6) C( 1) C( 7) H( 21) -179.8 .000 .000 .374 .000 .059 .000
N( 6) C( 5) C( 4) H( 16) -74.3 .000 .000 .374 .050 .059 -.001
N( 6) C( 5) C( 4) H( 17) 168.0 .000 .000 .374 .036 .059 -.001
N( 6) C( 10) C( 9) C( 8) -54.4 -.302 .696 .499 .232 .059 .000
N( 6) C( 10) C( 9) H( 12) -176.7 .000 .000 .374 .003 .059 .000
N( 6) C( 10) C( 9) H( 23) 66.2 .000 .000 .374 .010 .059 .000
C( 7) C( 1) C( 2) H( 14) 42.9 .000 .000 .010 .002 .270 -.007
C( 7) C( 1) N( 6) C( 10) -63.3 .958 -.155 .766 .576 .061 .000
C( 7) C( 8) C( 9) C( 10) 50.4 .185 .170 .520 .285 .059 .000
C( 7) C( 8) C( 9) H( 12) 172.7 .000 .000 .280 .010 .059 .000
C( 7) C( 8) C( 9) H( 23) -70.2 .000 .000 .280 .020 .059 .000
C( 8) C( 7) C( 1) H( 13) -60.4 .000 .000 .280 .000 .059 .000
C( 8) C( 9) C( 10) H( 24) -175.2 .000 .000 .280 .004 .059 .000
C( 8) C( 9) C( 10) H( 25) 68.0 .000 .000 .280 .012 .059 .000
C( 9) C( 8) C( 7) H( 20) 68.0 .000 .000 .280 .012 .059 .000
C( 9) C( 8) C( 7) H( 21) -175.2 .000 .000 .280 .004 .059 .000
C( 10) N( 6) C( 1) H( 13) 55.6 .072 -.012 .563 .055 .061 .000
C( 10) N( 6) C( 5) H( 18) -68.6 .072 -.012 .563 .067 .061 .000
C( 10) N( 6) C( 5) H( 19) 49.0 .072 -.012 .563 .099 .061 -.001
C( 10) C( 9) C( 8) H( 11) 172.6 .000 .000 .280 .010 .059 .000
C( 10) C( 9) C( 8) H( 22) -70.3 .000 .000 .280 .020 .059 .000
H( 11) C( 8) C( 7) H( 20) -54.1 .000 .000 .238 .006 .059 .000
H( 11) C( 8) C( 7) H( 21) 62.6 .000 .000 .238 .001 .059 .000
H( 11) C( 8) C( 9) H( 12) -65.1 .000 .000 .238 .004 .059 .000
H( 11) C( 8) C( 9) H( 23) 52.0 .000 .000 .238 .010 .059 .000
H( 12) C( 9) C( 8) H( 22) 52.0 .000 .000 .238 .010 .059 .000
H( 12) C( 9) C( 10) H( 24) 62.5 .000 .000 .238 .001 .059 .000
H( 12) C( 9) C( 10) H( 25) -54.3 .000 .000 .238 .005 .059 .000
H( 13) C( 1) C( 2) H( 14) -76.3 .000 .000 .580 .099 .270 -.006
H( 13) C( 1) C( 7) H( 20) 178.3 .000 .000 .238 .000 .059 .000
H( 13) C( 1) C( 7) H( 21) 60.9 .000 .000 .238 .000 .059 .000
H( 14) C( 2) C( 3) H( 15) -1.6 .000 11.500 .000 .009
H( 15) C( 3) C( 4) H( 16) -71.8 .000 .000 .580 .054 .270 -.002
H( 15) C( 3) C( 4) H( 17) 45.3 .000 .000 .580 .082 .270 -.002
H( 16) C( 4) C( 5) H( 18) 163.7 .000 .000 .238 .041 .059 -.002
H( 16) C( 4) C( 5) H( 19) 46.9 .000 .000 .238 .027 .059 -.001
H( 17) C( 4) C( 5) H( 18) 46.0 .000 .000 .238 .031 .059 -.001
H( 17) C( 4) C( 5) H( 19) -70.8 .000 .000 .238 .019 .059 -.001
H( 20) C( 7) C( 8) H( 22) -171.3 .000 .000 .238 .012 .059 .000
H( 21) C( 7) C( 8) H( 22) -54.5 .000 .000 .238 .005 .059 .000
H( 22) C( 8) C( 9) H( 23) 169.1 .000 .000 .238 .019 .059 .000
H( 23) C( 9) C( 10) H( 24) -54.6 .000 .000 .238 .005 .059 .000
H( 23) C( 9) C( 10) H( 25) -171.4 .000 .000 .238 .012 .059 .000

```

DIPOLE-DIPOLE INTERACTION ENERGY (DIELECTRIC CONSTANT = 1.50)

$$E = 14.388 \cdot \mu_1 \cdot \mu_2 \cdot (\cos X - 3 \cdot \cos A \cdot \cos B) / (R_{12}^3 \cdot \text{DIELC})$$

MU1 = BOND MOM OF BOND 1

MU2 = BOND MOM OF BOND 2

R12 = DISTANCE BETWEEN MID-POINTS OF TWO BONDS.

(ENERGIES LESS THAN 0.2 KCAL/MOL ARE NOT PRINTED.)

BOND(1)	MU1	BOND(2)	MU2	R12	E
C(1)- C(2)	.900	+ C(3)- C(4)	-.900	2.1421	1.0148
C(1)- C(2)	.900	+ C(3)- H(15)	-.600	2.3118	.5303
C(1)- C(2)	.900	+ C(5)- N(6)	.680	2.0840	-.6843
C(1)- C(2)	.900	+ N(6)- C(10)	-.680	2.4406	-.4288
C(1)- N(6)	.680	+ C(2)- H(14)	-.600	2.3427	-.2998
C(1)- N(6)	.680	+ C(3)- C(4)	-.900	2.4749	-.3688
C(2)- H(14)	-.600	+ C(3)- C(4)	-.900	2.2973	.5299
C(2)- H(14)	-.600	+ C(3)- H(15)	-.600	1.8916	.6381
C(3)- C(4)	-.900	+ C(5)- N(6)	.680	2.1327	.6370

=====

NORMAL MODE VIBRATIONAL ANALYSIS

=====

Molecular Shape : ASYMMETRIC ROTOR WITH KAPPA = -.690637
 Symmetry Point Group : C1
 Symmetry Number : 1
 Chirality : yes

0 FUNDAMENTAL NORMAL VIBRATIONAL FREQUENCIES
 (THEORETICALLY 69 VALUES)

Frequency : in 1/cm
 A(i) : IR intensity (vs,s,m,w,vw,-- or in 10**6 cm/mole)
 A(i) = -- : IR inactive

no	Frequency	Symmetry	A(i)
1.	3052.7	(A)	m
2.	3038.6	(A)	w
3.	2935.6	(A)	m
4.	2931.1	(A)	s
5.	2928.4	(A)	m
6.	2926.4	(A)	m
7.	2917.1	(A)	s
8.	2914.6	(A)	w
9.	2884.4	(A)	m
10.	2883.8	(A)	m
11.	2877.1	(A)	m
12.	2867.8	(A)	m
13.	2803.9	(A)	m
14.	2778.1	(A)	m
15.	2775.2	(A)	m
16.	1692.2	(A)	w
17.	1581.3	(A)	w
18.	1554.2	(A)	m
19.	1538.3	(A)	w
20.	1499.1	(A)	w
21.	1467.5	(A)	w
22.	1465.0	(A)	vw
23.	1460.2	(A)	w
24.	1454.6	(A)	w
25.	1444.1	(A)	w
26.	1427.6	(A)	w
27.	1408.2	(A)	w
28.	1405.1	(A)	w
29.	1379.4	(A)	w
30.	1377.5	(A)	w
31.	1359.5	(A)	m
32.	1308.3	(A)	w
33.	1293.9	(A)	w
34.	1241.8	(A)	w
35.	1227.0	(A)	vw
36.	1216.2	(A)	w
37.	1207.8	(A)	w
38.	1199.7	(A)	w
39.	1162.3	(A)	w
40.	1143.7	(A)	w
41.	1106.2	(A)	w
42.	1086.1	(A)	w
43.	1055.6	(A)	w
44.	1039.4	(A)	w
45.	1029.5	(A)	w
46.	999.8	(A)	w
47.	974.4	(A)	w
48.	952.4	(A)	w
49.	937.1	(A)	w

50.	928.6	(A)	w
51.	861.7	(A)	w
52.	852.2	(A)	w
53.	842.8	(A)	w
54.	817.8	(A)	w
55.	786.8	(A)	w
56.	681.9	(A)	m
57.	643.8	(A)	m
58.	552.1	(A)	w
59.	523.9	(A)	w
60.	469.2	(A)	w
61.	401.5	(A)	w
62.	392.0	(A)	w
63.	368.2	(A)	w
64.	343.0	(A)	w
65.	308.5	(A)	w
66.	270.1	(A)	w
67.	234.3	(A)	w
68.	148.5	(A)	w
69.	113.9	(A)	w
70.	(.0)	(t/r)	
71.	(.0)	(t/r)	
72.	(.0)	(t/r)	
73.	(.0)	(t/r)	
74.	(.0)	(t/r)	
75.	(.0)	(t/r)	

=====

STATISTICAL THERMODYNAMICS ANALYSIS

=====

Structure name : RINI
 Temperature : 298.16 K
 Symmetry number : 1
 Optical isomers : 2
 Zero Point Energy : 139.739 Kcal/mol

	ENERGY	ENTHALPY	ENTROPY	FREE ENERGY	HEAT CAPACITY
	(Kcal/mol)	(Kcal/mol)	(eu)	(Kcal/mol)	(cal/mol/deg)
Translational	.889	1.481	40.641	-10.636	4.967
Rotational	.889	.889	29.301	-7.848	2.980
Vibrational	143.450%	143.450%	19.935*	137.506%	30.348*
Potential	15.759#	15.759#	.000	15.759#	.000
Mixing	.000	.000	1.377	-.411	.000
Total	160.987	161.579	91.254	134.371	38.296

Enthalpy Function (H-Ho)/T = 20.39 cal/mol/deg
 Free Energy Function -(G-Ho)/T = 70.86 cal/mol/deg

% Includes zero point energy (ZPE).
 * Excludes contribution from frequencies lower than 40 (1/cm).
 # Includes steric energy (SE).
 Internal rotation contributions are not considered

This structure has 0 imaginary frequencies,
 0 free internal rotation (fir) frequencies
 (>= 0, < 10 /cm),
 0 restricted internal rotation (rir) frequencies
 (>= 10, < 40 /cm),
 6 zero frequencies, and
 69 real frequencies.

FINAL STERIC ENERGY IS 15.7593 KCAL/MOL.

COMPRESSION .6225
 BENDING 1.0733
 BEND-BEND -.0657

STRETCH-BEND .0896
 VANDERWAALS
 1,4 ENERGY 11.0016
 OTHER -.5665

TORSIONAL 1.9336
 TORSION-STRETCH -.0482
 DIPOLE-DIPOLE 1.7191
 CHARGE-DIPOLE .0000
 CHARGE-CHARGE .0000

COORDINATES TRANSLATED TO NEW ORIGIN WHICH IS CENTER OF MASS

C(1)	.00785	.69180	.42586	(1)
C(2)	1.30493	1.42458	.17893	(2)
C(3)	2.43701	.79929	-.16762	(2)
C(4)	2.49380	-.69509	-.33017	(1)
C(5)	1.25411	-1.36170	.27698	(1)
N(6)	.03738	-.66431	-.13287	(8)
C(7)	-1.17176	1.44547	-.21111	(1)
C(8)	-2.49835	.72848	.06565	(1)
C(9)	-2.41875	-.73932	-.36357	(1)
C(10)	-1.17127	-1.41065	.21628	(1)
H(11)	-3.33208	1.24060	-.46767	(5)
H(12)	-3.33497	-1.28412	-.04006	(5)
H(13)	-.14563	.64006	1.54175	(5)
H(14)	1.30209	2.52159	.29806	(5)
H(15)	3.35837	1.37521	-.35943	(5)
H(16)	2.56571	-.93644	-1.41508	(5)
H(17)	3.41198	-1.09463	.15692	(5)
H(18)	1.33086	-1.37562	1.40046	(5)
H(19)	1.21841	-2.42310	-.05767	(5)
H(20)	-1.01483	1.52943	-1.31116	(5)
H(21)	-1.22406	2.48461	.18767	(5)
H(22)	-2.72988	.78455	1.15456	(5)
H(23)	-2.38529	-.79717	-1.47606	(5)
H(24)	-1.10275	-2.44615	-.18705	(5)
H(25)	-1.26527	-1.50036	1.33460	(5)

MOMENT OF INERTIA WITH THE PRINCIPAL AXES

(1) UNIT = 10**(-39) GM*CM**2
 IX= 32.5396 IY= 76.5699 IZ= 101.7681

(2) UNIT = AU A**2
 IX= 195.9796 IY= 461.1653 IZ= 612.9286

DIPOLE MOMENT = .815 D

COMPONENTS WITH PRINCIPAL AXES

X = .2489 Y = .4641 Z = -.6224