VIB (V=0) 8	.112791D+01	.052275	.120367
VIB (V=0) 9	.110787D+01	.044490	.102443
VIB (V=0) 10	.109089D+01	.037783	.086998
VIB (V=0) 11	.107553D+01	.031622	.072811
VIB (V=0) 12	.107087D+01	.029736	.068470
VIB (V=0) 13	.105414D+01	.022899	.052727
ELECTRONIC	.100000D+01	.000000	.000000
TRANSLATIONAL	.589838D+08	7.770733	17.892773
ROTATIONAL	.298632D+06	5.475137	12.606969

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

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	.000000000	.000000000	-.000017302
2	7	.000000000	.000000000	.000142076
3	6	.000000000	.000000000	-.000260818
4	6	-.000177411	.000000000	.000099478
5	6	.000060648	.000000000	.000020378
6	6	.000177411	.000000000	.000099478
7	6	-.000060648	.000000000	.000020378
8	6	.000130343	.000000000	-.000046285
9	6	-.000130343	.000000000	-.000046285
10	6	.000000000	.000000000	-.000072739
11	1	-.000045658	.000000000	-.000022144
12	1	.000045658	.000000000	-.000022144
13	1	-.000003714	.000000000	.000045496
14	1	-.000004298	.000007986	-.000007196
15	1	-.000004298	-.000007986	-.000007196
16	1	.000003714	.000000000	.000045496
17	1	.000004298	-.000007986	-.000007196
18	1	.000004298	.000007986	-.000007196
19	1	.000000000	.000000000	.000043720

Cartesian Forces: Max .000260818 RMS .000064176
Internal Forces: Max .000138621 RMS .000026162

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Search for a local minimum.
Step number 1 out of a maximum of 114
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Second derivative matrix not updated -- analytic derivatives used.

Eigenvalues ---	-.00051	-.00021	.00199	.01195	.01251
Eigenvalues ---	.01509	.01521	.01652	.01848	.01942
Eigenvalues ---	.02118	.02291	.02315	.02545	.03554
Eigenvalues ---	.03762	.04526	.05358	.05444	.08606
Eigenvalues ---	.08615	.09944	.10058	.10117	.10264
Eigenvalues ---	.10862	.12106	.12297	.17659	.17802
Eigenvalues ---	.18453	.18606	.22873	.23716	.27950
Eigenvalues ---	.27990	.29392	.31447	.31455	.31858
Eigenvalues ---	.32279	.32690	.33813	.33964	.34228
Eigenvalues ---	.35496	.36767	.42036	.42978	.46360
Eigenvalues ---	.99872	1000.00000	1000.00000	1000.00000	1000.00000
Eigenvalues ---	1000.00000	1000.00000	1000.00000	1000.00000	1000.00000
Eigenvalues ---	1000.00000	1000.00000	1000.00000	1000.00000	1000.00000
Eigenvalues ---	1000.00000	1000.00000	1000.00000	1000.00000	1000.00000

```
     Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
 Eigenvalue    1 out of range, new value =      .000513 Eigenvector:
                              1
           R1                .00000
           R2                .00000
           R3                .00000
           R4                .00000
           R5                .00000
           R6                .00000
           R7                .00000
           R8                .00000
           R9                .00000
           R10               .00000
           R11               .00000
           R12               .00000
           R13               .00000
           R14               .00000
           R15               .00213
           R16              -.00213
           R17               .00000
           R18               .00000
           R19               .00213
           R20              -.00213
           R21               .00000
           A1                .00000
           A2                .00000
           A3                .00000
           A4                .00000
           A5                .00000
           A6                .00000
           A7                .00000
           A8                .00000
           A9                .00000
           A10               .00000
           A11               .00000
           A12               .00000
           A13               .00000
           A14               .00000
           A15               .00000
           A16               .00000
           A17               .00000
           A18               .00000
           A19               .00000
           A20               .00000
           A21               .00101
           A22              -.00687
           A23              -.00101
           A24               .00687
           A25               .00000
           A26               .00000
```

A27	.00000
A28	.00000
A29	.00000
A30	.00000
A31	.00101
A32	-.00687
A33	-.00101
A34	.00687
A35	.00000
A36	.00000
A37	.00000
D1	-.07313
D2	-.07313
D3	-.07313
D4	-.07313
D5	-.00153
D6	-.00153
D7	-.01357
D8	-.01357
D9	.00312
D10	.01486
D11	.00230
D12	.01404
D13	-.00153
D14	-.00153
D15	-.01357
D16	-.01357
D17	.00312
D18	.01486
D19	.00230
D20	.01404
D21	.20653
D22	.19419
D23	.21462
D24	.20227
D25	.21462
D26	.20227
D27	.20653
D28	.19419
D29	.21462
D30	.20227
D31	.21462
D32	.20227
D33	-.00163
D34	-.00080
D35	-.00163
D36	-.00080
D37	-.00163
D38	-.00080
D39	-.00163
D40	-.00080
D41	.19208
D42	.19208
D43	.19208
D44	-.20047
D45	-.20396
D46	-.20396

D47	.19208
D48	.19208
D49	.19208
D50	-.20047
D51	-.20396
D52	-.20396

Eigenvalue 2 out of range, new value = .000208 Eigenvector:

	1
R1	.00000
R2	.00000
R3	.00000
R4	.00000
R5	.00000
R6	.00000
R7	.00000
R8	.00000
R9	.00000
R10	.00000
R11	.00000
R12	.00000
R13	.00000
R14	.00000
R15	.00155
R16	-.00155
R17	.00000
R18	.00000
R19	-.00155
R20	.00155
R21	.00000
A1	.00000
A2	.00000
A3	.00000
A4	.00000
A5	.00000
A6	.00000
A7	.00000
A8	.00000
A9	.00000
A10	.00000
A11	.00000
A12	.00000
A13	.00000
A14	.00000
A15	.00000
A16	.00000
A17	.00000
A18	.00000
A19	.00000
A20	.00000
A21	-.00082
A22	-.00565
A23	.00082
A24	.00565
A25	.00000
A26	.00000
A27	.00000
A28	.00000

A29	.00000
A30	.00000
A31	.00082
A32	.00565
A33	-.00082
A34	-.00565
A35	.00000
A36	.00000
A37	.00000
D1	-.04212
D2	.04354
D3	-.04354
D4	.04212
D5	-.00753
D6	-.00606
D7	-.01974
D8	-.01827
D9	.00205
D10	.01395
D11	.00297
D12	.01487
D13	.00753
D14	.00606
D15	.01974
D16	.01827
D17	-.00205
D18	-.01395
D19	-.00297
D20	-.01487
D21	.14460
D22	.13209
D23	.15241
D24	.13990
D25	.15241
D26	.13990
D27	-.14460
D28	-.13209
D29	-.15241
D30	-.13990
D31	-.15241
D32	-.13990
D33	.00174
D34	.00081
D35	.00248
D36	.00155
D37	-.00174
D38	-.00081
D39	-.00248
D40	-.00155
D41	.12586
D42	.12489
D43	.53110
D44	-.13517
D45	-.14012
D46	-.14012
D47	-.12586
D48	-.12489

```
          D49          -.53110
          D50           .13517
          D51           .14012
          D52           .14012
 Angle between quadratic step and forces=  41.28 degrees.
 Linear search not attempted -- first point.
 Iteration  1 RMS(Cart)=    .00022479 RMS(Int)=    .00000003
 Iteration  2 RMS(Cart)=    .00000004 RMS(Int)=    .00000001
 TrRot=    .000000   .000000   .000000   .000000   .000000   .000000
```

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.25091	.00002	.00000	.00003	.00003	2.25094
R2	2.64281	-.00014	.00000	-.00049	-.00049	2.64231
R3	2.69260	-.00001	.00000	.00006	.00006	2.69265
R4	2.66338	-.00002	.00000	-.00007	-.00007	2.66331
R5	2.69260	-.00001	.00000	.00006	.00006	2.69265
R6	2.66338	-.00002	.00000	-.00007	-.00007	2.66331
R7	2.87284	.00009	.00000	.00049	.00049	2.87333
R8	2.87284	.00009	.00000	.00049	.00049	2.87333
R9	2.65484	-.00003	.00000	-.00006	-.00006	2.65478
R10	2.65484	-.00003	.00000	-.00006	-.00006	2.65478
R11	2.06935	-.00005	.00000	-.00016	-.00016	2.06920
R12	2.06935	-.00005	.00000	-.00016	-.00016	2.06920
R13	4.67834	.00002	.00000	.00085	.00085	4.67920
R14	2.07627	-.00004	.00000	-.00012	-.00012	2.07615
R15	2.08766	-.00001	.00000	-.00005	-.00005	2.08760
R16	2.08766	-.00001	.00000	-.00005	-.00005	2.08760
R17	4.67834	.00002	.00000	.00085	.00085	4.67920
R18	2.07627	-.00004	.00000	-.00012	-.00012	2.07615
R19	2.08766	-.00001	.00000	-.00005	-.00005	2.08760
R20	2.08766	-.00001	.00000	-.00005	-.00005	2.08760
R21	2.06766	.00004	.00000	.00013	.00013	2.06779
A1	2.07315	.00004	.00000	.00028	.00028	2.07343
A2	2.05041	.00005	.00000	.00036	.00036	2.05077
A3	2.07315	.00004	.00000	.00028	.00028	2.07343
A4	2.13689	-.00008	.00000	-.00056	-.00056	2.13633
A5	2.05041	.00005	.00000	.00036	.00036	2.05077
A6	2.13736	-.00002	.00000	.00001	.00001	2.13737
A7	2.09542	-.00003	.00000	-.00037	-.00037	2.09505
A8	2.13736	-.00002	.00000	.00001	.00001	2.13737
A9	2.09542	-.00003	.00000	-.00037	-.00037	2.09505
A10	2.11697	-.00001	.00000	-.00004	-.00004	2.11693
A11	2.11697	-.00001	.00000	-.00004	-.00004	2.11693
A12	2.09472	-.00001	.00000	-.00007	-.00007	2.09465
A13	2.07376	.00001	.00000	.00002	.00002	2.07378
A14	2.09245	.00000	.00000	.00003	.00003	2.09248
A15	2.07376	.00001	.00000	.00002	.00002	2.07378
A16	2.09245	.00000	.00000	.00003	.00003	2.09248
A17	1.67644	.00000	.00000	.00015	.00015	1.67658
A18	1.46516	.00000	.00000	-.00015	-.00015	1.46501
A19	1.96350	-.00004	.00000	-.00017	-.00017	1.96333
A20	1.78562	.00002	.00000	.00003	.00003	1.78564
A21	1.93164	.00001	.00000	.00000	.00000	1.93164
A22	1.88257	.00001	.00000	.00003	.00003	1.88260
A23	1.93164	.00001	.00000	.00000	.00000	1.93164
A24	1.88257	.00001	.00000	.00003	.00003	1.88260
A25	1.86838	.00000	.00000	.00012	.00012	1.86850

A26	1.67644	.00000	.00000	.00015	.00015	1.67658
A27	1.46516	.00000	.00000	-.00015	-.00015	1.46501
A28	2.93031	.00000	.00000	-.00030	-.00030	2.93002
A29	1.96350	-.00004	.00000	-.00017	-.00017	1.96333
A30	1.78562	.00002	.00000	.00003	.00003	1.78564
A31	1.93164	.00001	.00000	.00000	.00000	1.93164
A32	1.88257	.00001	.00000	.00003	.00003	1.88260
A33	1.93164	.00001	.00000	.00000	.00000	1.93164
A34	1.88257	.00001	.00000	.00003	.00003	1.88260
A35	1.86838	.00000	.00000	.00012	.00012	1.86850
A36	2.09423	.00000	.00000	.00004	.00004	2.09427
A37	2.09423	.00000	.00000	.00004	.00004	2.09427
D1	.00000	.00000	.00000	.00000	.00000	.00000
D2	3.14159	.00000	.00000	.00000	.00000	3.14159
D3	3.14159	.00000	.00000	.00000	.00000	3.14159
D4	.00000	.00000	.00000	.00000	.00000	.00000
D5	3.14159	.00000	.00000	.00000	.00000	3.14159
D6	.00000	.00000	.00000	.00000	.00000	.00000
D7	.00000	.00000	.00000	.00000	.00000	.00000
D8	3.14159	.00000	.00000	.00000	.00000	3.14159
D9	.00000	.00000	.00000	.00000	.00000	.00000
D10	3.14159	.00000	.00000	.00000	.00000	3.14159
D11	3.14159	.00000	.00000	.00000	.00000	3.14159
D12	.00000	.00000	.00000	.00000	.00000	.00000
D13	3.14159	.00000	.00000	.00000	.00000	3.14159
D14	.00000	.00000	.00000	.00000	.00000	.00000
D15	.00000	.00000	.00000	.00000	.00000	.00000
D16	3.14159	.00000	.00000	.00000	.00000	3.14159
D17	.00000	.00000	.00000	.00000	.00000	.00000
D18	3.14159	.00000	.00000	.00000	.00000	3.14159
D19	3.14159	.00000	.00000	.00000	.00000	3.14159
D20	.00000	.00000	.00000	.00000	.00000	.00000
D21	.00000	.00000	.00000	.00000	.00000	.00000
D22	3.14159	.00000	.00000	.00000	.00000	3.14159
D23	-2.10736	.00001	.00000	.00007	.00007	-2.10729
D24	1.03423	.00001	.00000	.00007	.00007	1.03430
D25	2.10736	-.00001	.00000	-.00007	-.00007	2.10729
D26	-1.03423	-.00001	.00000	-.00007	-.00007	-1.03430
D27	.00000	.00000	.00000	.00000	.00000	.00000
D28	3.14159	.00000	.00000	.00000	.00000	3.14159
D29	-2.10736	.00001	.00000	.00007	.00007	-2.10729
D30	1.03423	.00001	.00000	.00007	.00007	1.03430
D31	2.10736	-.00001	.00000	-.00007	-.00007	2.10729
D32	-1.03423	-.00001	.00000	-.00007	-.00007	-1.03430
D33	.00000	.00000	.00000	.00000	.00000	.00000
D34	3.14159	.00000	.00000	.00000	.00000	3.14159
D35	3.14159	.00000	.00000	.00000	.00000	3.14159
D36	.00000	.00000	.00000	.00000	.00000	.00000
D37	.00000	.00000	.00000	.00000	.00000	.00000
D38	3.14159	.00000	.00000	.00000	.00000	3.14159
D39	3.14159	.00000	.00000	.00000	.00000	3.14159
D40	.00000	.00000	.00000	.00000	.00000	.00000
D41	3.14159	.00000	.00000	.00000	.00000	3.14159
D42	.00000	.00000	.00000	.00000	.00000	.00000
D43	.00000	.00000	.00000	.00000	.00000	.00000
D44	.00000	.00000	.00000	.00000	.00000	.00000
D45	2.13531	.00000	.00000	-.00009	-.00009	2.13523

D46	-2.13531	.00000	.00000	.00009	.00009	-2.13523
D47	3.14159	.00000	.00000	.00000	.00000	3.14159
D48	.00000	.00000	.00000	.00000	.00000	.00000
D49	.00000	.00000	.00000	.00000	.00000	.00000
D50	.00000	.00000	.00000	.00000	.00000	.00000
D51	2.13531	.00000	.00000	-.00009	-.00009	2.13523
D52	-2.13531	.00000	.00000	.00009	.00009	-2.13523

Item		Value	Threshold	Converged?
Maximum	Force	.000139	.000450	YES
RMS	Force	.000026	.000300	YES
Maximum	Displacement	.000860	.001800	YES
RMS	Displacement	.000225	.001200	YES

Predicted change in Energy=-1.973279D-07
Optimization completed.
-- Stationary point found.

! Optimized Parameters !
! (Angstroms and Degrees) !

Name	Definition	Value	Derivative Info.
R1	R(2,1)	1.1911	-DE/DX = 0.
R2	R(3,2)	1.3985	-DE/DX = -0.0001
R3	R(4,3)	1.4249	-DE/DX = 0.
R4	R(5,4)	1.4094	-DE/DX = 0.
R5	R(6,3)	1.4249	-DE/DX = 0.
R6	R(7,6)	1.4094	-DE/DX = 0.
R7	R(8,4)	1.5202	-DE/DX = 0.0001
R8	R(9,6)	1.5202	-DE/DX = 0.0001
R9	R(10,5)	1.4049	-DE/DX = 0.
R10	R(10,7)	1.4049	-DE/DX = 0.
R11	R(11,5)	1.0951	-DE/DX = -0.0001
R12	R(12,7)	1.0951	-DE/DX = -0.0001
R13	R(13,2)	2.4757	-DE/DX = 0.
R14	R(13,8)	1.0987	-DE/DX = 0.
R15	R(14,8)	1.1047	-DE/DX = 0.
R16	R(15,8)	1.1047	-DE/DX = 0.
R17	R(16,2)	2.4757	-DE/DX = 0.
R18	R(16,9)	1.0987	-DE/DX = 0.
R19	R(17,9)	1.1047	-DE/DX = 0.
R20	R(18,9)	1.1047	-DE/DX = 0.
R21	R(19,10)	1.0942	-DE/DX = 0.
A1	A(2,3,4)	118.7825	-DE/DX = 0.
A2	A(3,4,5)	117.4796	-DE/DX = 0.0001
A3	A(2,3,6)	118.7825	-DE/DX = 0.
A4	A(4,3,6)	122.435	-DE/DX = -0.0001
A5	A(3,6,7)	117.4796	-DE/DX = 0.0001
A6	A(3,4,8)	122.4619	-DE/DX = 0.
A7	A(5,4,8)	120.0584	-DE/DX = 0.
A8	A(3,6,9)	122.4619	-DE/DX = 0.
A9	A(7,6,9)	120.0584	-DE/DX = 0.
A10	A(4,5,10)	121.2935	-DE/DX = 0.
A11	A(6,7,10)	121.2935	-DE/DX = 0.
A12	A(5,10,7)	120.0187	-DE/DX = 0.
A13	A(4,5,11)	118.8178	-DE/DX = 0.
A14	A(10,5,11)	119.8887	-DE/DX = 0.
A15	A(6,7,12)	118.8178	-DE/DX = 0.

```
! A16    A(10,7,12)            119.8887         -DE/DX =    0.              !
! A17    A(1,2,13)              96.0527         -DE/DX =    0.              !
! A18    A(3,2,13)              83.9473         -DE/DX =    0.              !
! A19    A(4,8,13)             112.5            -DE/DX =    0.              !
! A20    A(2,13,8)             102.3083         -DE/DX =    0.              !
! A21    A(4,8,14)             110.6748         -DE/DX =    0.              !
! A22    A(13,8,14)            107.8635         -DE/DX =    0.              !
! A23    A(4,8,15)             110.6748         -DE/DX =    0.              !
! A24    A(13,8,15)            107.8635         -DE/DX =    0.              !
! A25    A(14,8,15)            107.0503         -DE/DX =    0.              !
! A26    A(1,2,16)              96.0527         -DE/DX =    0.              !
! A27    A(3,2,16)              83.9473         -DE/DX =    0.              !
! A28    A(13,2,16)            167.8946         -DE/DX =    0.              !
! A29    A(6,9,16)             112.5            -DE/DX =    0.              !
! A30    A(2,16,9)             102.3083         -DE/DX =    0.              !
! A31    A(6,9,17)             110.6748         -DE/DX =    0.              !
! A32    A(16,9,17)            107.8635         -DE/DX =    0.              !
! A33    A(6,9,18)             110.6748         -DE/DX =    0.              !
! A34    A(16,9,18)            107.8635         -DE/DX =    0.              !
! A35    A(17,9,18)            107.0503         -DE/DX =    0.              !
! A36    A(5,10,19)            119.9906         -DE/DX =    0.              !
! A37    A(7,10,19)            119.9906         -DE/DX =    0.              !
! D1     D(4,3,2,13)             0.             -DE/DX =    0.              !
! D2     D(4,3,2,16)           180.             -DE/DX =    0.              !
! D3     D(6,3,2,13)           180.             -DE/DX =    0.              !
! D4     D(6,3,2,16)             0.             -DE/DX =    0.              !
! D5     D(5,4,3,2)            180.             -DE/DX =    0.              !
! D6     D(5,4,3,6)              0.             -DE/DX =    0.              !
! D7     D(8,4,3,2)              0.             -DE/DX =    0.              !
! D8     D(8,4,3,6)            180.             -DE/DX =    0.              !
! D9     D(10,5,4,3)             0.             -DE/DX =    0.              !
! D10    D(10,5,4,8)           180.             -DE/DX =    0.              !
! D11    D(11,5,4,3)           180.             -DE/DX =    0.              !
! D12    D(11,5,4,8)             0.             -DE/DX =    0.              !
! D13    D(7,6,3,2)            180.             -DE/DX =    0.              !
! D14    D(7,6,3,4)              0.             -DE/DX =    0.              !
! D15    D(9,6,3,2)              0.             -DE/DX =    0.              !
! D16    D(9,6,3,4)            180.             -DE/DX =    0.              !
! D17    D(10,7,6,3)             0.             -DE/DX =    0.              !
! D18    D(10,7,6,9)           180.             -DE/DX =    0.              !
! D19    D(12,7,6,3)           180.             -DE/DX =    0.              !
! D20    D(12,7,6,9)             0.             -DE/DX =    0.              !
! D21    D(13,8,4,3)             0.             -DE/DX =    0.              !
! D22    D(13,8,4,5)           180.             -DE/DX =    0.              !
! D23    D(14,8,4,3)          -120.7431         -DE/DX =    0.              !
! D24    D(14,8,4,5)            59.2569         -DE/DX =    0.              !
! D25    D(15,8,4,3)           120.7431         -DE/DX =    0.              !
! D26    D(15,8,4,5)           -59.2569         -DE/DX =    0.              !
! D27    D(16,9,6,3)             0.             -DE/DX =    0.              !
! D28    D(16,9,6,7)           180.             -DE/DX =    0.              !
! D29    D(17,9,6,3)          -120.7431         -DE/DX =    0.              !
! D30    D(17,9,6,7)            59.2569         -DE/DX =    0.              !
! D31    D(18,9,6,3)           120.7431         -DE/DX =    0.              !
! D32    D(18,9,6,7)           -59.2569         -DE/DX =    0.              !
! D33    D(7,10,5,4)             0.             -DE/DX =    0.              !
! D34    D(7,10,5,11)          180.             -DE/DX =    0.              !
! D35    D(19,10,5,4)          180.             -DE/DX =    0.              !
```

```
! D36    D(19,10,5,11)           0.             -DE/DX =    0.              !
! D37    D(5,10,7,6)             0.             -DE/DX =    0.              !
! D38    D(5,10,7,12)          180.             -DE/DX =    0.              !
! D39    D(19,10,7,6)          180.             -DE/DX =    0.              !
! D40    D(19,10,7,12)           0.             -DE/DX =    0.              !
! D41    D(8,13,2,1)           180.             -DE/DX =    0.              !
! D42    D(8,13,2,3)             0.             -DE/DX =    0.              !
! D43    D(8,13,2,16)            0.             -DE/DX =    0.              !
! D44    D(2,13,8,4)             0.             -DE/DX =    0.              !
! D45    D(2,13,8,14)          122.3443         -DE/DX =    0.              !
! D46    D(2,13,8,15)         -122.3443         -DE/DX =    0.              !
! D47    D(9,16,2,1)           180.             -DE/DX =    0.              !
! D48    D(9,16,2,3)             0.             -DE/DX =    0.              !
! D49    D(9,16,2,13)            0.             -DE/DX =    0.              !
! D50    D(2,16,9,6)             0.             -DE/DX =    0.              !
! D51    D(2,16,9,17)          122.3443         -DE/DX =    0.              !
! D52    D(2,16,9,18)         -122.3443         -DE/DX =    0.              !
--------------------------------------------------------------------------------
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

**********************************************************************

          Population analysis using the SCF density.

**********************************************************************

Orbital Symmetries:
      Occupied  (A1) (A1) (A1) (A1) (B2) (A1) (B2) (A1) (B2) (A1)
                (A1) (A1) (B2) (A1) (A1) (B2) (A1) (B2) (A1) (B2)
                (A1) (B1) (A1) (A2) (B2) (A1) (B1) (B2) (B2) (A1)
                (B1) (B2) (A1) (A2) (B1)
      Virtual   (B1) (A2) (B2) (A1) (A1) (B2) (B1) (B2) (B1) (A1)
                (A1) (A2) (A1) (B2) (B1) (B2) (B1) (A1) (A1) (B2)
                (A2) (B1) (A1) (B1) (A1) (A1) (B2) (B2) (A1) (B1)
                (A2) (B2) (A1) (B1) (A2) (B2) (A1) (B2) (A1) (B2)
                (A1) (A1) (B1) (A1) (B2) (B1) (B2) (A1) (A1) (B2)
                (A1) (B2) (A1) (B2) (A1) (B2) (A1) (A1) (A1) (B2)
                (B2) (A1) (B2) (A1) (B1) (A1) (B2) (B1) (A2) (B2)
                (A1) (A1) (A2) (B1) (B2) (B1) (B2) (A1) (A2) (B1)
                (A1) (B1) (B2) (A1) (B2) (A2) (A1) (A1) (B2) (B1)
                (B1) (B2) (A1) (A1) (B2) (B2) (A1) (A1) (B2) (A1)
                (B2) (A1) (B2) (A2) (A1) (A1) (B2) (B1) (A2) (A1)
                (B2) (A1) (B1) (B1) (A2) (A1) (A2) (A1) (B2) (A1)
                (B1) (B2) (A1) (B2) (A1) (B2) (A2) (A1) (B1) (B2)
                (A2) (A1) (A1) (B2) (A1) (A2) (B1) (A1) (B1) (A1)
                (B2) (B1) (A2) (B2) (A2) (A1) (A1) (B1) (B2) (A1)
                (B2) (A2) (A1) (B2) (A1) (B2) (A1) (B1) (B2) (A1)
                (B2) (A1) (A1) (A1) (A1) (B2) (A1) (B2) (A1) (A1)
                (B2) (A1) (A1)
 The electronic state is 1-A1.
Alpha  occ. eigenvalues --  -14.07580 -10.00044  -9.96709  -9.96458  -9.96458
Alpha  occ. eigenvalues --   -9.95078  -9.94720  -9.94718  -9.93818  -9.93818
Alpha  occ. eigenvalues --    -.87525   -.78557   -.71870   -.70405   -.65153
Alpha  occ. eigenvalues --    -.62089   -.58639   -.53280   -.50369   -.44152
Alpha  occ. eigenvalues --    -.43361   -.39490   -.38881   -.37540   -.37056
Alpha  occ. eigenvalues --    -.36611   -.35120   -.34221   -.32727   -.31996
```

Alpha occ. eigenvalues --	-.30691	-.29623	-.26299	-.22425	-.22408
Alpha virt. eigenvalues --	-.06914	-.05435	-.02362	-.01273	.00274
Alpha virt. eigenvalues --	.00435	.00925	.02427	.02614	.03031
Alpha virt. eigenvalues --	.04132	.04956	.04977	.06515	.06671
Alpha virt. eigenvalues --	.07213	.07847	.08362	.08862	.09971
Alpha virt. eigenvalues --	.10316	.10786	.11053	.11887	.12367
Alpha virt. eigenvalues --	.12697	.14662	.14872	.15207	.15582
Alpha virt. eigenvalues --	.15839	.16007	.16667	.17553	.18513
Alpha virt. eigenvalues --	.18576	.20064	.20142	.20429	.21209
Alpha virt. eigenvalues --	.21564	.22300	.23163	.23641	.24104
Alpha virt. eigenvalues --	.24783	.25273	.25411	.25796	.26686
Alpha virt. eigenvalues --	.27301	.28243	.29080	.31087	.32187
Alpha virt. eigenvalues --	.32665	.33364	.35908	.37021	.39636
Alpha virt. eigenvalues --	.41008	.48294	.50249	.53302	.61715
Alpha virt. eigenvalues --	.61969	.62266	.63719	.64500	.64616
Alpha virt. eigenvalues --	.65746	.67005	.68337	.68445	.68679
Alpha virt. eigenvalues --	.70549	.71436	.73124	.73257	.75628
Alpha virt. eigenvalues --	.76243	.78981	.82170	.83725	.83952
Alpha virt. eigenvalues --	.86426	.87317	.88529	.89077	.92396
Alpha virt. eigenvalues --	.94331	.96891	.97252	1.00907	1.01305
Alpha virt. eigenvalues --	1.04216	1.07549	1.10708	1.10949	1.11768
Alpha virt. eigenvalues --	1.13944	1.16391	1.16740	1.17625	1.21554
Alpha virt. eigenvalues --	1.24053	1.24674	1.26275	1.32099	1.32914
Alpha virt. eigenvalues --	1.33977	1.34066	1.35742	1.40014	1.41518
Alpha virt. eigenvalues --	1.42702	1.46714	1.50440	1.52797	1.66405
Alpha virt. eigenvalues --	1.68401	1.68625	1.72431	1.76520	1.79099
Alpha virt. eigenvalues --	1.79459	1.80540	1.81070	1.84404	1.84460
Alpha virt. eigenvalues --	1.86722	1.89314	1.95970	1.98649	2.03424
Alpha virt. eigenvalues --	2.05421	2.08322	2.08870	2.10903	2.15063
Alpha virt. eigenvalues --	2.17955	2.21661	2.23035	2.26550	2.26777
Alpha virt. eigenvalues --	2.28058	2.29182	2.32347	2.34888	2.43456
Alpha virt. eigenvalues --	2.45360	2.53959	2.54732	2.57624	2.64785
Alpha virt. eigenvalues --	2.68503	2.70878	2.70900	2.81983	2.88761
Alpha virt. eigenvalues --	3.11067	3.18537	3.39068	4.10022	4.15361
Alpha virt. eigenvalues --	4.17207	4.20458	4.24467	4.27976	4.33859
Alpha virt. eigenvalues --	4.38278	4.41107	4.70018		

Condensed to atoms (all electrons):

		1	2	3	4	5	6
1	C	5.996020	.850749	.173591	-.390577	.196901	-.390577
2	N	.850749	6.893821	-1.801288	.792869	-.384972	.792869
3	C	.173591	-1.801288	40.055905	-18.423201	7.303275	-18.423201
4	C	-.390577	.792869	-18.423201	23.446598	-6.914055	9.249218
5	C	.196901	-.384972	7.303275	-6.914055	13.864330	-7.123725
6	C	-.390577	.792869	-18.423201	9.249218	-7.123725	23.446598
7	C	.196901	-.384972	7.303275	-7.123725	2.919168	-6.914055
8	C	-.164375	.168974	-1.746045	.879510	-1.619819	.496696
9	C	-.164375	.168974	-1.746045	.496696	-.281853	.879510
10	C	-.071014	.100833	-5.714147	3.238493	-1.537247	3.238493
11	H	.000570	-.000645	.173376	-.096350	.340407	-.024234
12	H	.000570	-.000645	.173376	-.024234	.035753	-.096350
13	H	.001098	.016432	-.181203	.021488	.129220	-.082141
14	H	.001275	.000455	.175171	-.157660	-.126992	.006833
15	H	.001275	.000455	.175171	-.157660	-.126992	.006833
16	H	.001098	.016432	-.181203	-.082141	.010854	.021488
17	H	.001275	.000455	.175171	.006833	.004150	-.157660
18	H	.001275	.000455	.175171	.006833	.004150	-.157660
19	H	-.000099	.000105	-.013443	.052472	-.078733	.052472

		7	8	9	10	11	12
1	C	.196901	-.164375	-.164375	-.071014	.000570	.000570
2	N	-.384972	.168974	.168974	.100833	-.000645	-.000645
3	C	7.303275	-1.746045	-1.746045	-5.714147	.173376	.173376
4	C	-7.123725	.879510	.496696	3.238493	-.096350	-.024234
5	C	2.919168	-1.619819	-.281853	-1.537247	.340407	.035753
6	C	-6.914055	.496696	.879510	3.238493	-.024234	-.096350
7	C	13.864330	-.281853	-1.619819	-1.537247	.035753	.340407
8	C	-.281853	7.700177	-.085898	.118740	-.040961	.001793
9	C	-1.619819	-.085898	7.700177	.118740	.001793	-.040961
10	C	-1.537247	.118740	.118740	7.426635	-.123251	-.123251
11	H	.035753	-.040961	.001793	-.123251	.568518	-.000184
12	H	.340407	.001793	-.040961	-.123251	-.000184	.568518
13	H	.010854	.428617	-.003436	-.004378	.000130	.000000
14	H	.004150	.444367	-.000551	-.021724	.001072	.000000
15	H	.004150	.444367	-.000551	-.021724	.001072	.000000
16	H	.129220	-.003436	.428617	-.004378	.000000	.000130
17	H	-.126992	-.000551	.444367	-.021724	.000000	.001072
18	H	-.126992	-.000551	.444367	-.021724	.000000	.001072
19	H	-.078733	-.000708	-.000708	.352269	-.005026	-.005026

		13	14	15	16	17	18
1	C	.001098	.001275	.001275	.001098	.001275	.001275
2	N	.016432	.000455	.000455	.016432	.000455	.000455
3	C	-.181203	.175171	.175171	-.181203	.175171	.175171
4	C	.021488	-.157660	-.157660	-.082141	.006833	.006833
5	C	.129220	-.126992	-.126992	.010854	.004150	.004150
6	C	-.082141	.006833	.006833	.021488	-.157660	-.157660
7	C	.010854	.004150	.004150	.129220	-.126992	-.126992
8	C	.428617	.444367	.444367	-.003436	-.000551	-.000551
9	C	-.003436	-.000551	-.000551	.428617	.444367	.444367
10	C	-.004378	-.021724	-.021724	-.004378	-.021724	-.021724
11	H	.000130	.001072	.001072	.000000	.000000	.000000
12	H	.000000	.000000	.000000	.000130	.001072	.001072
13	H	.481312	-.025020	-.025020	.000000	.000000	.000000
14	H	-.025020	.504702	-.031924	.000000	.000000	.000000
15	H	-.025020	-.031924	.504702	.000000	.000000	.000000
16	H	.000000	.000000	.000000	.481312	-.025020	-.025020
17	H	.000000	.000000	.000000	-.025020	.504702	-.031924
18	H	.000000	.000000	.000000	-.025020	-.031924	.504702
19	H	.000002	-.000002	-.000002	.000002	-.000002	-.000002

		19
1	C	-.000099
2	N	.000105
3	C	-.013443
4	C	.052472
5	C	-.078733
6	C	.052472
7	C	-.078733
8	C	-.000708
9	C	-.000708
10	C	.352269
11	H	-.005026
12	H	-.005026
13	H	.000002
14	H	-.000002
15	H	-.000002
16	H	.000002

```
17  H    -.000002
18  H    -.000002
19  H     .560992
Total atomic charges:
              1
 1  C    -.241581
 2  N    -.231356
 3  C   -1.653704
 4  C    1.178594
 5  C    -.613819
 6  C    1.178594
 7  C    -.613819
 8  C    -.739044
 9  C    -.739044
10  C     .607608
11  H     .167960
12  H     .167960
13  H     .232046
14  H     .225848
15  H     .225848
16  H     .232046
17  H     .225848
18  H     .225848
19  H     .164168
Sum of Mulliken charges=     .00000
Atomic charges with hydrogens summed into heavy atoms:
              1
 1  C    -.241581
 2  N    -.231356
 3  C   -1.653704
 4  C    1.178594
 5  C    -.445859
 6  C    1.178594
 7  C    -.445859
 8  C    -.055303
 9  C    -.055303
10  C     .771775
11  H     .000000
12  H     .000000
13  H     .000000
14  H     .000000
15  H     .000000
16  H     .000000
17  H     .000000
18  H     .000000
19  H     .000000
Sum of Mulliken charges=     .00000
Electronic spatial extent (au):  <R**2>=  1416.1361
Charge=      .0000 electrons
Dipole moment (Debye):
   X=      .0000    Y=      .0000    Z=    -3.7515  Tot=     3.7515
Quadrupole moment (Debye-Ang):
  XX=   -62.6108   YY=   -52.3265   ZZ=   -70.6796
  XY=      .0000   XZ=      .0000   YZ=      .0000
Octapole moment (Debye-Ang**2):
 XXX=      .0000  YYY=      .0000  ZZZ=   -74.3335  XYY=      .0000
 XXY=      .0000  XXZ=     1.6368  XZZ=      .0000  YZZ=      .0000
```

```
 YYZ=    -4.8430  XYZ=      .0000
Hexadecapole moment (Debye-Ang**3):
XXXX=   -89.2304 YYYY=  -918.7693 ZZZZ= -1192.0179 XXXY=      .0000
XXXZ=      .0000 YYYX=      .0000 YYYZ=      .0000 ZZZX=      .0000
ZZZY=      .0000 XXYY=  -170.6239 XXZZ=  -198.0694 YYZZ=  -318.3993
XXYZ=      .0000 YYXZ=      .0000 ZZXY=      .0000
N-N= 4.666328469088D+02 E-N=-1.865535287537D+03  KE= 3.988457422475D+02
Symmetry A1    KE= 2.676298677961D+02
Symmetry A2    KE= 4.265439485176D+00
Symmetry B1    KE= 9.181333853912D+00
Symmetry B2    KE= 1.177691011123D+02
 Exact polarizability:  67.694    .000 130.125    .000    .000 149.498
Approx polarizability: 114.430    .000 233.478    .000    .000 299.839
1\1\ PUCC-LIVELY\Freq\RBLYP\6-31+G(d)\C9H9N1\ZAVARINE\23-Sep-1997\0\\#
 BLYP 6-31+G* FREQ GEOM=CHECKPOINT GUESS=CHECKPOINT\\xylil frequencies
\\0,1\C,0.,0.,-3.0484067567\N,0.,0.,-1.8572748195\C,0.,0.,-0.458762440
9\C,1.2488240846,0.,0.2272875495\C,1.2167778377,0.,1.6363224256\C,-1.2
488240846,0.,0.2272875495\C,-1.2167778377,0.,1.6363224256\C,2.58158955
16,0.,-0.5040609342\C,-2.5815895516,0.,-0.5040609342\C,0.,0.,2.3385642
927\H,2.1639674972,0.,2.1858465434\H,-2.1639674972,0.,2.1858465434\H,2
.4618704203,0.,-1.5962316123\H,3.1777140383,-0.8883413897,-0.228496476
1\H,3.1777140383,0.8883413897,-0.2284964761\H,-2.4618704203,0.,-1.5962
316123\H,-3.1777140383,0.8883413897,-0.2284964761\H,-3.1777140383,-0.8
883413897,-0.2284964761\H,0.,0.,3.4327207175\\Version=IBM-RS6000-G94Re
vD.2\State=1-A1\HF=-402.9300856\RMSD=8.620e-09\RMSF=6.418e-05\Dipole=0
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0.,0.,0.0972617,0.,0.,0.,0.417871,0.2813151,0.,-0.0386556,0.,-0.026934
,0.,-0.1546352,0.,0.0281169,-0.0330786,0.,0.1015648,0.,-0.1494399,0.,0
.2013529,0.,-0.0783811,0.2813151,0.,0.0386556,0.,-0.026934,0.,0.154635
2,0.,0.0281169,-0.0330786,0.,-0.1015648,0.,-0.1494399,0.,-0.2013529,0.
,-0.0783811,-0.0448212,0.,0.0515835,0.,0.1254788,0.,-0.0338016,0.,0.06
06278,-0.0448212,0.,-0.0515835,0.,0.1254788,0.,0.0338016,0.,0.0606278,
0.0875648,0.,0.,0.,-0.1175648,0.,0.,0.,0.0915782,-0.0833532,0.,-0.0891
863,0.,0.1250606,0.,-0.0666087,0.,0.013795,-0.0833532,0.,0.0891863,0.,
0.1250606,0.,0.0666087,0.,0.013795,0.0579552,0.,-0.0335113,0.,0.076832
6,0.,0.0568975,0.,-0.0761186,-0.0438924,0.0584362,0.017535,0.1101191,-
0.0416261,0.0314933,0.0115771,0.0583426,0.0457507,-0.0438924,-0.058436
2,0.017535,-0.1101191,-0.0416261,-0.0314933,0.0115771,-0.0583426,0.045
7507,0.0579552,0.,0.0335113,0.,0.0768326,0.,-0.0568975,0.,-0.0761186,-
0.0438924,0.0584362,-0.017535,0.1101191,-0.0416261,-0.0314933,-0.01157
71,-0.0583426,0.0457507,-0.0438924,-0.0584362,-0.017535,-0.1101191,-0.
0416261,0.0314933,-0.0115771,0.0583426,0.0457507,0.0551881,0.,0.,0.,0.
1335862,0.,0.,0.,-0.1333131\Polar=130.1247385,0.,67.6942984,0.,0.,149.
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0.,-0.07901118,0.,0.,0.59524969,0.,0.00923323,0.,0.,-0.05305709,0.,0.,
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000850,0.00002781,0.,-0.00012170,0.,0.00005111,-0.00000850,0.00002781,
-0.00005111,-0.00000850,-0.00002781,0.,0.02355228,0.,0.,0.00005724,0.,
0.,-0.00021084,0.,0.,0.00077638,0.00285184,0.,0.00091356,-0.00218053,0
.,-0.01152088,-0.00285183,0.,0.00091356,0.00218053,0.,-0.01152088,-0.0
0047938,0.,-0.00062367,0.00047938,0.,-0.00062367,0.,0.,-0.32042476,0.0
0025221,0.,0.00088030,-0.00025221,0.,0.00088030,0.00025404,0.,-0.00011
527,0.00003589,-0.00002455,-0.00000480,0.00003589,0.00002455,-0.000004
80,-0.00025404,0.,-0.00011527,-0.00003589,0.00002455,-0.00000480,-0.00
003589,-0.00002455,-0.00000480,0.,0.,0.34075306\\0.,0.,0.00001730,0.,0
.,-0.00014208,0.,0.,0.00026082,0.00017741,0.,-0.00009948,-0.00006065,0
.,-0.00002038,-0.00017741,0.,-0.00009948,0.00006065,0.,-0.00002038,-0.
00013034,0.,0.00004628,0.00013034,0.,0.00004628,0.,0.,0.00007274,0.000
04566,0.,0.00002214,-0.00004566,0.,0.00002214,0.00000371,0.,-0.0000455
0,0.00000430,-0.00000799,0.00000720,0.00000430,0.00000799,0.00000720,-
0.00000371,0.,-0.00004550,-0.00000430,0.00000799,0.00000720,-0.0000043
0,-0.00000799,0.00000720,0.,0.,-0.00004372\\\@

IF I HAVE SEEN FARTHER, IT IS BY STANDING ON THE
SHOULDERS OF GIANTS. -- SIR ISAAC NEWTON

Job cpu time: 1 days 18 hours 30 minutes 54.0 seconds.
File lengths (MBytes): RWF= 105 Int= 0 D2E= 0 Chk= 4 Scr= 1
Normal termination of Gaussian 94

```
 Entering Gaussian System, Link 0=g94
AIX runner 1 4 000047578900
 Initial command:
 /usr/share/apps2/g94-D2/l1.exe /usr/share/scratch10/zav/g94-26120.inp
-scrdir=/usr/share/scratch10/zav/
 Entering Link 1 = /usr/share/apps2/g94-D2/l1.exe PID=     17676.

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 G. A. Petersson, J. A. Montgomery, K. Raghavachari,
 M. A. Al-Laham, V. G. Zakrzewski, J. V. Ortiz, J. B. Foresman,
 J. Cioslowski, B. B. Stefanov, A. Nanayakkara, M. Challacombe,
 C. Y. Peng, P. Y. Ayala, W. Chen, M. W. Wong, J. L. Andres,
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E. S. Replogle, R. Gomperts, R. L. Martin, D. J. Fox,
J. S. Binkley, D. J. Defrees, J. Baker, J. P. Stewart,
M. Head-Gordon, C. Gonzalez, and J. A. Pople,
Gaussian, Inc., Pittsburgh PA, 1995.

******************************************
Gaussian 94:  IBM-RS6000-G94RevD.2  1-Mar-1996
                22-Feb-1999
******************************************
%CHK=tertmod
Default route:  MaxDisk=600MB
------------------------------------
# BLYP 6-31+G(d) OPT FREQ symm=loose
------------------------------------
1/14=-1,18=20,26=3,38=1/1,3;
2/9=110,12=2,17=4,18=3/2;
3/5=1,6=6,7=11,11=2,25=1,30=1/1,2,3;
4//1;
5/5=2,38=4,42=42/2;
6/7=2,8=2,9=2,10=2,28=1/1;
7//1,2,3,16;
1/14=-1/3(1);
99//99;
2/9=110/2;
3/5=1,6=6,7=11,11=2,25=1,30=1/1,2,3;
4/5=5,16=2/1;
5/5=2,38=4,42=42/2;
7//1,2,3,16;
1/14=-1/3(-5);
2/9=110/2;
3/5=1,6=6,7=11,11=2,25=1,30=1,39=1/1,3;
6/7=2,8=2,9=2,10=2,28=1/1;
99/9=1/99;
----
tert
----
Symbolic Z-matrix:
   Charge = 0 Multiplicity = 1
C1
N2    1     R1
C3    2     R2        1     a3
C4    3     R3        2     A1        1     0.        0
C5    3     R3        2     A1        1     -d2       0
C6    3     R3        2     A1        1     d2        0
H7    4     R4        3     A2        2     d3        0
H8    4     R4        3     A4        2     d1        0
H9    4     R4        3     A5        2     -d1       0
H10   5     R4        3     A2        2     d3        0
H11   5     R4        3     A4        2     d1        0
H12   5     R4        3     A5        2     -d1       0
H13   6     R4        3     A2        2     d3        0
H14   6     R4        3     A4        2     d1        0
H15   6     R4        3     A5        2     -d1       0
      Variables:
 R1                    1.17973
 R2                    1.3891
 R3                    1.5
```

```
R4                      1.08
A1                    109.5
A2                    109.5
d1                     40.
a3                    179.999
d2                    120.
d3                    179.999
a4                    109.5
a5                    109.5

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Initialization pass.
                          ----------------------------
                          !    Initial Parameters    !
                          ! (Angstroms and Degrees)  !
-------------------------                            -------------------------
! Name  Definition              Value          Derivative Info.                !
--------------------------------------------------------------------------------
! R1    R(2,1)                  1.1797         estimate D2E/DX2                !
! R2    R(3,2)                  1.3891         estimate D2E/DX2                !
! R3    R(4,3)                  1.5            estimate D2E/DX2                !
! R4    R(5,3)                  1.5            estimate D2E/DX2                !
! R5    R(6,3)                  1.5            estimate D2E/DX2                !
! R6    R(7,4)                  1.08           estimate D2E/DX2                !
! R7    R(8,4)                  1.08           estimate D2E/DX2                !
! R8    R(9,4)                  1.08           estimate D2E/DX2                !
! R9    R(10,5)                 1.08           estimate D2E/DX2                !
! R10   R(11,5)                 1.08           estimate D2E/DX2                !
! R11   R(12,5)                 1.08           estimate D2E/DX2                !
! R12   R(13,6)                 1.08           estimate D2E/DX2                !
! R13   R(14,6)                 1.08           estimate D2E/DX2                !
! R14   R(15,6)                 1.08           estimate D2E/DX2                !
! A1    L(1,2,3)                180.           estimate D2E/DX2                !
! A2    L(1,2,3)                179.999        estimate D2E/DX2                !
! A3    A(2,3,4)                109.5          estimate D2E/DX2                !
! A4    A(2,3,5)                109.5          estimate D2E/DX2                !
! A5    A(4,3,5)                109.4424       estimate D2E/DX2                !
! A6    A(2,3,6)                109.5          estimate D2E/DX2                !
! A7    A(4,3,6)                109.4424       estimate D2E/DX2                !
! A8    A(5,3,6)                109.4424       estimate D2E/DX2                !
! A9    A(3,4,7)                109.5          estimate D2E/DX2                !
! A10   A(3,4,8)                109.5          estimate D2E/DX2                !
! A11   A(7,4,8)                124.6979       estimate D2E/DX2                !
! A12   A(3,4,9)                109.5          estimate D2E/DX2                !
! A13   A(7,4,9)                124.6993       estimate D2E/DX2                !
! A14   A(8,4,9)                 74.5899       estimate D2E/DX2                !
! A15   A(3,5,10)               109.5          estimate D2E/DX2                !
! A16   A(3,5,11)               109.5          estimate D2E/DX2                !
! A17   A(10,5,11)              124.6979       estimate D2E/DX2                !
! A18   A(3,5,12)               109.5          estimate D2E/DX2                !
! A19   A(10,5,12)              124.6993       estimate D2E/DX2                !
! A20   A(11,5,12)               74.5899       estimate D2E/DX2                !
! A21   A(3,6,13)               109.5          estimate D2E/DX2                !
! A22   A(3,6,14)               109.5          estimate D2E/DX2                !
! A23   A(13,6,14)              124.6979       estimate D2E/DX2                !
! A24   A(3,6,15)               109.5          estimate D2E/DX2                !
```

! A25	A(13,6,15)	124.6993	estimate D2E/DX2 !
! A26	A(14,6,15)	74.5899	estimate D2E/DX2 !
! D1	D(7,4,3,2)	179.999	estimate D2E/DX2 !
! D2	D(7,4,3,5)	-59.9658	estimate D2E/DX2 !
! D3	D(7,4,3,6)	59.9638	estimate D2E/DX2 !
! D4	D(8,4,3,2)	40.	estimate D2E/DX2 !
! D5	D(8,4,3,5)	160.0352	estimate D2E/DX2 !
! D6	D(8,4,3,6)	-80.0352	estimate D2E/DX2 !
! D7	D(9,4,3,2)	-40.	estimate D2E/DX2 !
! D8	D(9,4,3,5)	80.0352	estimate D2E/DX2 !
! D9	D(9,4,3,6)	-160.0352	estimate D2E/DX2 !
! D10	D(10,5,3,2)	179.999	estimate D2E/DX2 !
! D11	D(10,5,3,4)	59.9638	estimate D2E/DX2 !
! D12	D(10,5,3,6)	-59.9658	estimate D2E/DX2 !
! D13	D(11,5,3,2)	40.	estimate D2E/DX2 !
! D14	D(11,5,3,4)	-80.0352	estimate D2E/DX2 !
! D15	D(11,5,3,6)	160.0352	estimate D2E/DX2 !
! D16	D(12,5,3,2)	-40.	estimate D2E/DX2 !
! D17	D(12,5,3,4)	-160.0352	estimate D2E/DX2 !
! D18	D(12,5,3,6)	80.0352	estimate D2E/DX2 !
! D19	D(13,6,3,2)	179.999	estimate D2E/DX2 !
! D20	D(13,6,3,4)	-59.9658	estimate D2E/DX2 !
! D21	D(13,6,3,5)	59.9638	estimate D2E/DX2 !
! D22	D(14,6,3,2)	40.	estimate D2E/DX2 !
! D23	D(14,6,3,4)	160.0352	estimate D2E/DX2 !
! D24	D(14,6,3,5)	-80.0352	estimate D2E/DX2 !
! D25	D(15,6,3,2)	-40.	estimate D2E/DX2 !
! D26	D(15,6,3,4)	80.0352	estimate D2E/DX2 !
! D27	D(15,6,3,5)	-160.0352	estimate D2E/DX2 !

Trust Radius=3.00D-01 FncErr=1.00D-07 GrdErr=1.00D-06
Number of steps in this run= 77 maximum allowed number of steps= 100.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	.000000	.000000	.000000
2	7	.000000	.000000	1.179730
3	6	.000024	.000000	2.568830
4	6	1.413995	.000000	3.069516
5	6	-.706948	-1.224527	3.069553
6	6	-.706948	1.224527	3.069553
7	1	1.414014	.000018	4.149516
8	1	2.014145	.654392	2.454705
9	1	2.014145	-.654392	2.454705
10	1	-.706914	-1.224536	4.149553
11	1	-.440319	-2.071477	2.454748
12	1	-1.573759	-1.417085	2.454768
13	1	-.706945	1.224518	4.149553
14	1	-1.573759	1.417085	2.454768
15	1	-.440319	2.071477	2.454748

Distance matrix (angstroms):

1	2	3	4	5

1	C	.000000					
2	N	1.179730	.000000				
3	C	2.568830	1.389100	.000000			
4	C	3.379543	2.360227	1.500000	.000000		
5	C	3.379556	2.360227	1.500000	2.449054	.000000	
6	C	3.379556	2.360227	1.500000	2.449054	2.449054	
7	H	4.383824	3.289234	2.120833	1.080000	2.676623	
8	H	3.242003	2.471956	2.120833	1.080000	3.363439	
9	H	3.242003	2.471956	2.120833	1.080000	2.847356	
10	H	4.383834	3.289234	2.120833	2.676607	1.080000	
11	H	3.242019	2.471956	2.120833	2.847356	1.080000	
12	H	3.242026	2.471956	2.120833	3.363439	1.080000	
13	H	4.383834	3.289234	2.120833	2.676623	2.676607	
14	H	3.242026	2.471956	2.120833	3.363439	2.847356	
15	H	3.242019	2.471956	2.120833	2.847356	3.363439	
		6	7	8	9	10	
6	C	.000000					
7	H	2.676607	.000000				
8	H	2.847356	1.913307	.000000			
9	H	3.363439	1.913320	1.308783	.000000		
10	H	2.676623	2.449054	3.715782	3.256030	.000000	
11	H	3.363439	3.256053	3.668072	2.834171	1.913307	
12	H	2.847356	3.715796	4.142954	3.668072	1.913320	
13	H	1.080000	2.449054	3.256053	3.715796	2.449054	
14	H	1.080000	3.715782	3.668072	4.142954	3.256053	
15	H	1.080000	3.256030	2.834171	3.668072	3.715796	
		11	12	13	14	15	
11	H	.000000					
12	H	1.308783	.000000				
13	H	3.715782	3.256030	.000000			
14	H	3.668072	2.834171	1.913307	.000000		
15	H	4.142954	3.668072	1.913320	1.308783	.000000	

Stoichiometry C5H9N
Framework group C3V[C3(CNC),3SGV(CH),X(H6)]
Deg. of freedom 9
Full point group C3V NOp 6
Largest Abelian subgroup CS NOp 2
Largest concise Abelian subgroup CS NOp 2

Standard orientation:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	.000000	.000000	2.306519
2	7	.000000	.000000	1.126789
3	6	.000000	.000000	-.262311
4	6	.000000	1.413973	-.762997
5	6	-1.224536	-.706986	-.762997
6	6	1.224536	-.706986	-.762997
7	1	.000000	1.413992	-1.842997
8	1	.654366	2.014131	-.148186
9	1	-.654366	2.014131	-.148186
10	1	-1.224553	-.706996	-1.842997
11	1	-2.071471	-.440368	-.148186
12	1	-1.417106	-1.573763	-.148186
13	1	1.224553	-.706996	-1.842997
14	1	1.417106	-1.573763	-.148186

```
 15          1           2.071471    -.440368    -.148186
---------------------------------------------------------------
Rotational constants (GHZ):      4.8066971      3.0465288      3.0465288
Isotopes: C-12,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
Standard basis: 6-31+G(d) (6D, 7F)
There are    85 symmetry adapted basis functions of A'  symmetry.
There are    47 symmetry adapted basis functions of A"  symmetry.
Crude estimate of integral set expansion from redundant integrals=1.123.
Integral buffers will be    262144 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
  132 basis functions      228 primitive gaussians
   23 alpha electrons       23 beta electrons
      nuclear repulsion energy       235.8351997636 Hartrees.
One-electron integrals computed using PRISM.
The smallest eigenvalue of the overlap matrix is  2.373D-05
Projected INDO Guess.
Initial guess orbital symmetries:
      Occupied  (A1) (A1) (A1) (?A) (?A) (?A) (A1) (A1) (?B) (?B)
                (A1) (A1) (E) (E) (E) (E) (A1) (E) (E) (?C) (A1)
                (?D) (?D)
      Virtual   (?E) (?E) (?F) (?F) (A1) (E) (E) (?G) (A1) (?H)
                (E) (E) (?H) (E) (E) (A1) (A1) (E) (E) (A1) (A1)
                (E) (E) (A1) (A1) (E) (E) (A1) (?A) (?A) (A1)
                (?A) (E) (E) (A1) (E) (E) (A1) (A1) (E) (E) (A1)
                (A1) (E) (E) (A1) (?I) (?I) (?I) (E) (E) (?G)
                (?E) (?E) (?F) (?H) (?E) (?E) (?H) (A1) (E) (E)
                (A1) (?B) (?D) (?B) (?E) (?I) (?E) (?E) (?E) (?E)
                (?I) (?E) (?H) (?E) (?E) (?E) (?E) (?G) (?H)
                (?C) (?E) (?D) (?F) (?E) (?E) (?E) (?E) (?H) (?E)
                (?F) (?E) (?E) (?E) (?E) (?D) (?C) (?D) (?E) (?C)
                (?B) (?E) (?E) (?E) (?C) (?F) (?C)
Requested convergence on RMS density matrix=1.00D-08 within  64 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Integral accuracy reduced to 1.0D-05 until final iterations.
Initial convergence to 1.0D-05 achieved.  Increase integral accuracy.
SCF Done:  E(RB-LYP) =  -250.423706447     A.U. after   16 cycles
           Convg  =     .5424D-08             -V/T =  2.0070
           S**2   =    .0000

*********************************************************************

          Population analysis using the SCF density.

*********************************************************************

Orbital Symmetries:
      Occupied  (A1) (A1) (A1) (E) (E) (A1) (A1) (?A) (?B) (?B)
                (A1) (?A) (E) (E) (?C) (?C) (A1) (E) (E) (?D)
                (?D) (?D) (A1)
      Virtual   (A1) (E) (E) (A1) (E) (E) (?A) (E) (E) (?E) (?E)
                (A1) (?F) (?F) (A2) (E) (E) (?B) (A1) (E) (E)
                (A1) (A1) (?G) (?G) (?B) (E) (E) (A1) (E) (E)
                (?H) (?H) (A1) (A1) (E) (E) (?A) (A1) (A1) (E)
                (E) (A1) (E) (E) (?I) (?I) (E) (E) (?D) (?A) (E)
                (E) (A1) (?I) (A1) (E) (E) (E) (E) (A1) (E) (E)
                (?B) (?H) (?H) (?A) (?H) (?H) (A1) (A1) (?F) (?F)
```

```
                (A1) (?I) (A1) (?F) (?D) (?D) (?B) (?D) (?D) (?G)
                (?I) (?G) (?H) (?G) (A1) (?D) (?F) (?B) (?D) (?F)
                (?G) (?C) (?D) (?G) (?I) (?B) (?A) (?E) (?E) (A1)
                (A1) (?H) (?F) (A1) (A1) (?I)
 Unable to determine electronic state: an orbital has unidentified symmetry.
 Alpha  occ. eigenvalues --  -14.06785  -9.99850  -9.96289  -9.93017  -9.93017
 Alpha  occ. eigenvalues --   -9.93017   -.88657   -.76452   -.65794   -.65794
 Alpha  occ. eigenvalues --    -.60666   -.50845   -.41744   -.41744   -.40906
 Alpha  occ. eigenvalues --    -.40906   -.38975   -.30898   -.30898   -.27443
 Alpha  occ. eigenvalues --    -.27443   -.27001   -.25990
 Alpha virt. eigenvalues --    -.01631   -.01606   -.01606    .00866    .01379
 Alpha virt. eigenvalues --     .01379    .03468    .05146    .05146    .05210
 Alpha virt. eigenvalues --     .05210    .06975    .07964    .07964    .09915
 Alpha virt. eigenvalues --     .10117    .10117    .10179    .12951    .13605
 Alpha virt. eigenvalues --     .13605    .14110    .17098    .17275    .17275
 Alpha virt. eigenvalues --     .20324    .22962    .22962    .24055    .25351
 Alpha virt. eigenvalues --     .25351    .25672    .25672    .28162    .29444
 Alpha virt. eigenvalues --     .31247    .31247    .32094    .38227    .43345
 Alpha virt. eigenvalues --     .58445    .58445    .59399    .64299    .64299
 Alpha virt. eigenvalues --     .71716    .71716    .74930    .74930    .75050
 Alpha virt. eigenvalues --     .75765    .80989    .80989    .83362    .86127
 Alpha virt. eigenvalues --     .87616    .90500    .90500    .93920    .93920
 Alpha virt. eigenvalues --     .97670   1.03113   1.03113   1.03683   1.08804
 Alpha virt. eigenvalues --    1.08804   1.16042   1.19565   1.19565   1.23420
 Alpha virt. eigenvalues --    1.41051   1.42124   1.42124   1.57038   1.57038
 Alpha virt. eigenvalues --    1.68599   1.69632   1.70572   1.70572   1.87848
 Alpha virt. eigenvalues --    1.87848   1.95167   1.95167   1.95740   1.98611
 Alpha virt. eigenvalues --    1.98611   2.03368   2.09897   2.09897   2.11113
 Alpha virt. eigenvalues --    2.11214   2.11214   2.11350   2.18741   2.35882
 Alpha virt. eigenvalues --    2.35882   2.44919   2.53541   2.62489   2.62489
 Alpha virt. eigenvalues --    2.84918   2.84918   3.30248   4.10378   4.20723
 Alpha virt. eigenvalues --    4.20723   4.23873   4.32965   4.73336
          Condensed to atoms (all electrons):
                 1         2         3         4         5         6
  1  C    5.330517   .857389  -.290103   .022276   .022276   .022276
  2  N     .857389  6.644324  -.838295   .181806   .181806   .181806
  3  C    -.290103  -.838295  9.816887  -.740316  -.740316  -.740316
  4  C     .022276   .181806  -.740316  6.041302  -.057212  -.057212
  5  C     .022276   .181806  -.740316  -.057212  6.041302  -.057212
  6  C     .022276   .181806  -.740316  -.057212  -.057212  6.041302
  7  H    -.001393  -.007142   .069325   .366044  -.037320  -.037320
  8  H     .001470   .007048  -.118866   .401687   .050173  -.024088
  9  H     .001470   .007048  -.118866   .401687  -.024088   .050173
 10  H    -.001393  -.007142   .069325  -.037320   .366044  -.037320
 11  H     .001470   .007048  -.118866  -.024088   .401687   .050173
 12  H     .001470   .007048  -.118866   .050173   .401687  -.024088
 13  H    -.001393  -.007142   .069325  -.037320  -.037320   .366044
 14  H     .001470   .007048  -.118866   .050173  -.024088   .401687
 15  H     .001470   .007048  -.118866  -.024088   .050173   .401687
                 7         8         9        10        11        12
  1  C    -.001393   .001470   .001470  -.001393   .001470   .001470
  2  N    -.007142   .007048   .007048  -.007142   .007048   .007048
  3  C     .069325  -.118866  -.118866   .069325  -.118866  -.118866
  4  C     .366044   .401687   .401687  -.037320  -.024088   .050173
  5  C    -.037320   .050173  -.024088   .366044   .401687   .401687
  6  C    -.037320  -.024088   .050173  -.037320   .050173  -.024088
  7  H     .476187  -.012794  -.012794   .002508  -.000189   .000058
```

8	H	-.012794	.578953	-.084263	.000058	.000206	-.000375
9	H	-.012794	-.084263	.578953	-.000189	.001323	.000206
10	H	.002508	.000058	-.000189	.476187	-.012794	-.012794
11	H	-.000189	.000206	.001323	-.012794	.578953	-.084263
12	H	.000058	-.000375	.000206	-.012794	-.084263	.578953
13	H	.002508	-.000189	.000058	.002508	.000058	-.000189
14	H	.000058	.000206	-.000375	-.000189	.000206	.001323
15	H	-.000189	.001323	.000206	.000058	-.000375	.000206

		13	14	15
1	C	-.001393	.001470	.001470
2	N	-.007142	.007048	.007048
3	C	.069325	-.118866	-.118866
4	C	-.037320	.050173	-.024088
5	C	-.037320	-.024088	.050173
6	C	.366044	.401687	.401687
7	H	.002508	.000058	-.000189
8	H	-.000189	.000206	.001323
9	H	.000058	-.000375	.000206
10	H	.002508	-.000189	.000058
11	H	.000058	.000206	-.000375
12	H	-.000189	.001323	.000206
13	H	.476187	-.012794	-.012794
14	H	-.012794	.578953	-.084263
15	H	-.012794	-.084263	.578953

Total atomic charges:

		1
1	C	.030729
2	N	-.229697
3	C	.037679
4	C	-.537591
5	C	-.537591
6	C	-.537591
7	H	.192451
8	H	.199452
9	H	.199452
10	H	.192451
11	H	.199452
12	H	.199452
13	H	.192451
14	H	.199452
15	H	.199452

Sum of Mulliken charges= .00000

Atomic charges with hydrogens summed into heavy atoms:

		1
1	C	.030729
2	N	-.229697
3	C	.037679
4	C	.053763
5	C	.053763
6	C	.053763
7	H	.000000
8	H	.000000
9	H	.000000
10	H	.000000
11	H	.000000
12	H	.000000
13	H	.000000

```
14  H      .000000
15  H      .000000
Sum of Mulliken charges=     .00000
Electronic spatial extent (au):  <R**2>=    560.7107
Charge=       .0000 electrons
Dipole moment (Debye):
   X=       .0000    Y=       .0000    Z=     -3.3526  Tot=      3.3526
Quadrupole moment (Debye-Ang):
  XX=    -39.0071   YY=    -39.0071   ZZ=    -47.3429
  XY=       .0000   XZ=       .0000   YZ=       .0000
Octapole moment (Debye-Ang**2):
 XXX=       .0000  YYY=      5.7626  ZZZ=    -45.6789  XYY=       .0000
 XXY=     -5.7626  XXZ=      1.7671  XZZ=       .0000  YZZ=       .0000
 YYZ=      1.7671  XYZ=       .0000
Hexadecapole moment (Debye-Ang**3):
XXXX=   -221.5947 YYYY=   -221.5947 ZZZZ=   -478.4505 XXXY=       .0000
XXXZ=       .0000 YYYX=       .0000 YYYZ=      -.1229 ZZZX=       .0000
ZZZY=       .0000 XXYY=    -73.8649 XXZZ=   -106.5310 YYZZ=   -106.5310
XXYZ=       .1229 YYXZ=       .0000 ZZXY=       .0000
N-N= 2.358351997636D+02 E-N=-1.051140032242D+03  KE= 2.486939555028D+02
Symmetry A'    KE= 2.022112177701D+02
Symmetry A"    KE= 4.648273773264D+01
***** Axes restored to original set *****
-------------------------------------------------------------------
Center     Atomic                   Forces (Hartrees/Bohr)
Number     Number              X              Y              Z
-------------------------------------------------------------------
   1          6           .000000000     .000000000    -.016177234
   2          7           .000000000     .000000000    -.026607545
   3          6           .000000000     .000000000     .015650936
   4          6           .019354833     .000000252    -.037222922
   5          6          -.009677198    -.016761903    -.037222922
   6          6          -.009677635     .016761651    -.037222922
   7          1           .019477645     .000000254     .007251294
   8          1          -.000044397     .061229653     .019508121
   9          1          -.000042802    -.061229654     .019508121
  10          1          -.009738603    -.016868262     .007251294
  11          1           .053048633    -.030576378     .019508121
  12          1          -.053005035     .030651894     .019508121
  13          1          -.009739042     .016868009     .007251294
  14          1          -.053004236    -.030653275     .019508121
  15          1           .053047837     .030577759     .019508121
-------------------------------------------------------------------
Cartesian Forces:  Max      .061229654 RMS      .026902622
Internal  Forces:  Max      .042784779 RMS      .020035821

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Search for a local minimum.
Step number   1 out of a maximum of  77
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Second derivative matrix not updated -- first step.
    Eigenvalues ---     .00766    .00766    .00766    .04557    .04557
    Eigenvalues ---     .04557    .05182    .06590    .06590    .06590
    Eigenvalues ---     .06904    .06904    .16000    .16000    .16000
    Eigenvalues ---     .16000    .16000    .16000    .16000    .16000
    Eigenvalues ---     .16000    .17707    .17707    .25000    .25000
```

```
    Eigenvalues ---     .32377    .32377    .32377    .35994    .35994
    Eigenvalues ---     .35994    .35996    .35996    .35996    .35996
    Eigenvalues ---     .35996    .35996    .47476   1.157051000.00000
    Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
    Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
    Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
    Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
    Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
    Eigenvalues --- 1000.000001000.00000
RFO step:  Lambda=-1.07939418D-01.
Linear search not attempted -- first point.
Maximum step size (    .300) exceeded in Quadratic search.
   -- Step size scaled by    .419
Iteration  1 RMS(Cart)=   .03409263 RMS(Int)=   .00083266
Iteration  2 RMS(Cart)=   .00067748 RMS(Int)=   .00009549
Iteration  3 RMS(Cart)=   .00003461 RMS(Int)=   .00008758
Iteration  4 RMS(Cart)=   .00000163 RMS(Int)=   .00008755
TrRot=   .000000   .000000   .000000   .000000   .000000   .000000
```

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.22937	.01618	.00000	.00536	.00536	2.23473
R2	2.62502	.04278	.00000	.03078	.03078	2.65580
R3	2.83459	.03954	.00000	.03840	.03840	2.87299
R4	2.83459	.03954	.00000	.03840	.03840	2.87299
R5	2.83459	.03954	.00000	.03840	.03840	2.87299
R6	2.04090	.00725	.00000	.00650	.00650	2.04740
R7	2.04090	.02597	.00000	.02327	.02325	2.06415
R8	2.04090	.02597	.00000	.02327	.02325	2.06415
R9	2.04090	.00725	.00000	.00650	.00650	2.04740
R10	2.04090	.02597	.00000	.02327	.02325	2.06415
R11	2.04090	.02597	.00000	.02327	.02325	2.06415
R12	2.04090	.00725	.00000	.00650	.00650	2.04740
R13	2.04090	.02597	.00000	.02327	.02325	2.06415
R14	2.04090	.02597	.00000	.02327	.02325	2.06415
A1	3.14159	.00000	.00000	.00000	.00000	3.14159
A2	3.14158	.00000	.00000	.00000	.00002	3.14159
A3	1.91114	-.00074	.00000	-.00193	-.00195	1.90919
A4	1.91114	-.00074	.00000	-.00193	-.00195	1.90919
A5	1.91013	.00074	.00000	.00194	.00195	1.91208
A6	1.91114	-.00074	.00000	-.00193	-.00195	1.90919
A7	1.91013	.00074	.00000	.00194	.00195	1.91208
A8	1.91013	.00074	.00000	.00194	.00195	1.91208
A9	1.91114	.01376	.00000	.01143	.01118	1.92232
A10	1.91114	-.00663	.00000	-.00728	-.00740	1.90374
A11	2.17639	-.01922	.00000	-.03755	-.03771	2.13868
A12	1.91114	-.00663	.00000	-.00728	-.00740	1.90374
A13	2.17641	-.01922	.00000	-.03755	-.03774	2.13868
A14	1.30184	.04123	.00000	.09472	.09466	1.39650
A15	1.91114	.01376	.00000	.01143	.01118	1.92232
A16	1.91114	-.00663	.00000	-.00728	-.00740	1.90374
A17	2.17639	-.01922	.00000	-.03755	-.03771	2.13868
A18	1.91114	-.00663	.00000	-.00728	-.00740	1.90374
A19	2.17641	-.01922	.00000	-.03755	-.03774	2.13868
A20	1.30184	.04123	.00000	.09472	.09466	1.39650
A21	1.91114	.01376	.00000	.01143	.01118	1.92232
A22	1.91114	-.00663	.00000	-.00728	-.00740	1.90374
A23	2.17639	-.01922	.00000	-.03755	-.03771	2.13868

A24	1.91114	-.00663	.00000	-.00728	-.00740	1.90374
A25	2.17641	-.01922	.00000	-.03755	-.03774	2.13868
A26	1.30184	.04123	.00000	.09472	.09466	1.39650
D1	3.14158	.00000	.00000	.00000	.00002	3.14159
D2	-1.04660	-.00090	.00000	-.00237	-.00237	-1.04897
D3	1.04657	.00090	.00000	.00237	.00241	1.04897
D4	.69813	.02074	.00000	.05001	.04995	.74808
D5	2.79314	.01984	.00000	.04764	.04756	2.84070
D6	-1.39688	.02164	.00000	.05238	.05234	-1.34454
D7	-.69813	-.02074	.00000	-.05001	-.04995	-.74808
D8	1.39688	-.02164	.00000	-.05238	-.05234	1.34454
D9	-2.79314	-.01984	.00000	-.04764	-.04756	-2.84070
D10	3.14158	.00000	.00000	.00000	.00002	3.14159
D11	1.04657	.00090	.00000	.00237	.00241	1.04897
D12	-1.04660	-.00090	.00000	-.00237	-.00237	-1.04897
D13	.69813	.02074	.00000	.05001	.04995	.74808
D14	-1.39688	.02164	.00000	.05238	.05234	-1.34454
D15	2.79314	.01984	.00000	.04764	.04756	2.84070
D16	-.69813	-.02074	.00000	-.05001	-.04995	-.74808
D17	-2.79314	-.01984	.00000	-.04764	-.04756	-2.84070
D18	1.39688	-.02164	.00000	-.05238	-.05234	1.34454
D19	3.14158	.00000	.00000	.00000	.00002	3.14159
D20	-1.04660	-.00090	.00000	-.00237	-.00237	-1.04897
D21	1.04657	.00090	.00000	.00237	.00241	1.04897
D22	.69813	.02074	.00000	.05001	.04995	.74808
D23	2.79314	.01984	.00000	.04764	.04756	2.84070
D24	-1.39688	.02164	.00000	.05238	.05234	-1.34454
D25	-.69813	-.02074	.00000	-.05001	-.04995	-.74808
D26	1.39688	-.02164	.00000	-.05238	-.05234	1.34454
D27	-2.79314	-.01984	.00000	-.04764	-.04756	-2.84070

Item		Value	Threshold	Converged?
Maximum	Force	.042785	.000450	NO
RMS	Force	.020036	.000300	NO
Maximum	Displacement	.090426	.001800	NO
RMS	Displacement	.034035	.001200	NO

Predicted change in Energy=-4.629237D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	.000000	.000000	-2.334983
2	7	.000000	.000000	-1.152416
3	6	.000000	.000000	.252972
4	6	1.434104	.000019	.757672
5	6	-.717036	-1.241980	.757672
6	6	-.717068	1.241961	.757672
7	1	1.448333	.000019	1.841017
8	1	2.022037	.702243	.162410
9	1	2.022056	-.702190	.162410
10	1	-.724150	-1.254302	1.841017
11	1	-.402858	-2.102257	.162410
12	1	-1.619143	-1.400056	.162410
13	1	-.724183	1.254284	1.841017
14	1	-1.619179	1.400014	.162410

15	1	-.402913	2.102247	.162410

Distance matrix (angstroms):

		1	2	3	4	5
1	C	.000000				
2	N	1.182567	.000000			
3	C	2.587955	1.405388	.000000		
4	C	3.408983	2.388533	1.520321	.000000	
5	C	3.408983	2.388533	1.520321	2.483940	.000000
6	C	3.408983	2.388533	1.520321	2.483940	2.483940
7	H	4.420027	3.325403	2.149314	1.083438	2.721216
8	H	3.289187	2.512080	2.142424	1.092301	3.411284
9	H	3.289187	2.512080	2.142424	1.092301	2.854528
10	H	4.420027	3.325403	2.149314	2.721216	1.083438
11	H	3.289187	2.512080	2.142424	2.854528	1.092301
12	H	3.289187	2.512080	2.142424	3.411284	1.092301
13	H	4.420027	3.325403	2.149314	2.721216	2.721216
14	H	3.289187	2.512080	2.142424	3.411284	2.854528
15	H	3.289187	2.512080	2.142424	2.854528	3.411284

		6	7	8	9	10
6	C	.000000				
7	H	2.721216	.000000			
8	H	2.854528	1.907872	.000000		
9	H	3.411284	1.907872	1.404434	.000000	
10	H	2.721216	2.508586	3.766608	3.265608	.000000
11	H	3.411284	3.265608	3.707471	2.800070	1.907872
12	H	2.854528	3.766608	4.204504	3.707471	1.907872
13	H	1.083438	2.508586	3.265608	3.766608	2.508586
14	H	1.092301	3.766608	3.707471	4.204504	3.265608
15	H	1.092301	3.265608	2.800070	3.707471	3.766608

		11	12	13	14	15
11	H	.000000				
12	H	1.404434	.000000			
13	H	3.766608	3.265608	.000000		
14	H	3.707471	2.800070	1.907872	.000000	
15	H	4.204504	3.707471	1.907872	1.404434	.000000

Stoichiometry C5H9N
Framework group C3V[C3(CNC),3SGV(CH),X(H6)]
Deg. of freedom 9
Full point group C3V NOp 6
Largest Abelian subgroup CS NOp 2
Largest concise Abelian subgroup CS NOp 2

Standard orientation:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	.000000	.000000	2.325779
2	7	.000000	.000000	1.143212
3	6	.000000	.000000	-.262176
4	6	.000000	1.434104	-.766876
5	6	-1.241970	-.717052	-.766876
6	6	1.241970	-.717052	-.766876
7	1	.000000	1.448333	-1.850220
8	1	.702217	2.022046	-.171614
9	1	-.702217	2.022046	-.171614
10	1	-1.254293	-.724166	-1.850220

11	1	-2.102252	-.402886	-.171614
12	1	-1.400035	-1.619161	-.171614
13	1	1.254293	-.724166	-1.850220
14	1	1.400035	-1.619161	-.171614
15	1	2.102252	-.402886	-.171614

```
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      4.6756447      2.9856920      2.9856920
 Isotopes: C-12,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
 Standard basis: 6-31+G(d) (6D, 7F)
 There are    85 symmetry adapted basis functions of A'  symmetry.
 There are    47 symmetry adapted basis functions of A"  symmetry.
 Crude estimate of integral set expansion from redundant integrals=1.123.
 Integral buffers will be    262144 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   132 basis functions      228 primitive gaussians
    23 alpha electrons       23 beta electrons
       nuclear repulsion energy       233.2441293932 Hartrees.
 One-electron integrals computed using PRISM.
 The smallest eigenvalue of the overlap matrix is  2.543D-05
 Initial guess read from the read-write file:
 Initial guess orbital symmetries:
       Occupied  (A1) (A1) (A1) (E) (E) (A1) (A1) (?A) (?B) (?B)
                 (A1) (?A) (E) (E) (E) (E) (A1) (E) (E) (?C) (?C)
                 (?C) (A1)
       Virtual   (A1) (E) (E) (A1) (E) (E) (?A) (E) (E) (?D) (?D)
                 (A1) (A2) (A2) (A2) (E) (E) (?B) (A1) (E) (E)
                 (A1) (?B) (?E) (?E) (?B) (E) (E) (?F) (E) (E)
                 (?G) (?G) (A1) (A1) (E) (E) (?A) (?A) (A1) (E)
                 (E) (A1) (E) (E) (?H) (?H) (E) (E) (?C) (?B) (E)
                 (E) (A1) (?H) (A1) (E) (E) (E) (E) (A1) (E) (E)
                 (?B) (?G) (?G) (?A) (?G) (?G) (A1) (A1) (A2) (?G)
                 (?F) (?H) (A1) (A2) (?C) (?C) (?B) (?C) (?C) (?E)
                 (?H) (?G) (?G) (?E) (?B) (?C) (A2) (?B) (?C) (A2)
                 (?E) (?C) (?C) (?E) (?H) (?B) (?A) (?D) (?D) (A1)
                 (A1) (?G) (A2) (A1) (A1) (?H)
  Requested convergence on RMS density matrix=1.00D-08 within  64 cycles.
  Requested convergence on MAX density matrix=1.00D-06.
  Integral accuracy reduced to 1.0D-05 until final iterations.
  Initial convergence to 1.0D-05 achieved.  Increase integral accuracy.
  SCF Done:  E(RB-LYP) =  -250.463710690     A.U. after   14 cycles
             Convg  =      .7642D-09             -V/T =  2.0082
             S**2   =      .0000
  ***** Axes restored to original set *****
  -------------------------------------------------------------------
  Center     Atomic                   Forces (Hartrees/Bohr)
  Number     Number              X              Y              Z
  -------------------------------------------------------------------
     1          6           .000000000     .000000000    -.010660591
     2          7           .000000000     .000000000    -.017592687
     3          6           .000000000     .000000000     .017982546
     4          6           .017143458     .000000223    -.044579734
     5          6          -.008571536    -.014846782    -.044579734
     6          6          -.008571922     .014846559    -.044579734
     7          1           .015627376     .000000204     .005304382
     8          1          -.003789546     .044705194     .021349464
     9          1          -.003788381    -.044705293     .021349464
```

10	1	-.007813512	-.013533806	.005304382
11	1	.040610607	-.019070754	.021349464
12	1	-.036821729	.025633481	.021349464
13	1	-.007813864	.013533603	.005304382
14	1	-.036821061	-.025634440	.021349464
15	1	.040610110	.019071812	.021349464

Cartesian Forces: Max .044705293 RMS .022715446
Internal Forces: Max .033020167 RMS .014819565

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Search for a local minimum.
Step number 2 out of a maximum of 77
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Update second derivatives using information from points 1 2
Trust test= 8.64D+00 RLast= 3.00D-01 DXMaxT set to 4.24D-01
Maximum step size (.424) exceeded in linear search.
-- Step size scaled by .360
-- Skip Quadratic or steepest descent search.
Quartic linear search produced a step of 1.41477.
Steepest descent instead of Quadratic search.
Iteration 1 RMS(Cart)= .04463860 RMS(Int)= .00163836
Iteration 2 RMS(Cart)= .00139038 RMS(Int)= .00025750
Iteration 3 RMS(Cart)= .00010511 RMS(Int)= .00022760
Iteration 4 RMS(Cart)= .00000686 RMS(Int)= .00022739
TrRot= .000000 .000000 -.000006 .000000 .000000 .000000

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.23473	.01066	.00758	-.00533	.00226	2.23698
R2	2.65580	.02825	.04355	-.01342	.03013	2.68593
R3	2.87299	.02490	.05433	-.01506	.03927	2.91226
R4	2.87299	.02490	.05433	-.01506	.03927	2.91226
R5	2.87299	.02490	.05433	-.01506	.03927	2.91226
R6	2.04740	.00551	.00919	-.00046	.00873	2.05614
R7	2.06415	.01507	.03289	-.01313	.01976	2.08391
R8	2.06415	.01507	.03289	-.01313	.01976	2.08391
R9	2.04740	.00551	.00919	-.00046	.00873	2.05614
R10	2.06415	.01507	.03289	-.01313	.01976	2.08391
R11	2.06415	.01507	.03289	-.01313	.01976	2.08391
R12	2.04740	.00551	.00919	-.00046	.00873	2.05614
R13	2.06415	.01507	.03289	-.01313	.01976	2.08391
R14	2.06415	.01507	.03289	-.01313	.01976	2.08391
A1	3.14159	.00000	.00000	.00000	.00000	3.14159
A2	3.14159	.00000	.00002	.00000	.00000	3.14159
A3	1.90919	-.00070	-.00276	-.00033	-.00308	1.90611
A4	1.90919	-.00070	-.00276	-.00033	-.00308	1.90611
A5	1.91208	.00069	.00275	.00032	.00306	1.91514
A6	1.90919	-.00070	-.00276	-.00033	-.00308	1.90611
A7	1.91208	.00069	.00275	.00032	.00306	1.91514
A8	1.91208	.00069	.00275	.00032	.00306	1.91514
A9	1.92232	.01072	.01582	-.00026	.01499	1.93731
A10	1.90374	-.00416	-.01046	.00254	-.00831	1.89543
A11	2.13868	-.01633	-.05336	-.00370	-.05752	2.08116
A12	1.90374	-.00416	-.01046	.00254	-.00831	1.89543
A13	2.13868	-.01633	-.05339	-.00370	-.05752	2.08116
A14	1.39650	.03302	.13392	.00343	.13702	1.53352

A15	1.92232	.01072	.01582	-.00026	.01499	1.93731
A16	1.90374	-.00416	-.01046	.00254	-.00831	1.89543
A17	2.13868	-.01633	-.05336	-.00370	-.05752	2.08116
A18	1.90374	-.00416	-.01046	.00254	-.00831	1.89543
A19	2.13868	-.01633	-.05339	-.00370	-.05752	2.08116
A20	1.39650	.03302	.13392	.00343	.13702	1.53352
A21	1.92232	.01072	.01582	-.00026	.01499	1.93731
A22	1.90374	-.00416	-.01046	.00254	-.00831	1.89543
A23	2.13868	-.01633	-.05336	-.00370	-.05752	2.08116
A24	1.90374	-.00416	-.01046	.00254	-.00831	1.89543
A25	2.13868	-.01633	-.05339	-.00370	-.05752	2.08116
A26	1.39650	.03302	.13392	.00343	.13702	1.53352
D1	3.14159	.00000	.00002	.00000	.00000	3.14159
D2	-1.04897	-.00085	-.00336	-.00041	-.00379	-1.05276
D3	1.04897	.00085	.00340	.00041	.00379	1.05276
D4	.74808	.01692	.07067	.00257	.07323	.82131
D5	2.84070	.01607	.06729	.00215	.06944	2.91014
D6	-1.34454	.01778	.07405	.00298	.07702	-1.26752
D7	-.74808	-.01692	-.07067	-.00257	-.07323	-.82131
D8	1.34454	-.01778	-.07405	-.00298	-.07702	1.26752
D9	-2.84070	-.01607	-.06729	-.00215	-.06944	-2.91014
D10	3.14159	.00000	.00002	.00000	.00000	3.14159
D11	1.04897	.00085	.00340	.00041	.00379	1.05276
D12	-1.04897	-.00085	-.00336	-.00041	-.00379	-1.05276
D13	.74808	.01692	.07067	.00257	.07323	.82131
D14	-1.34454	.01778	.07405	.00298	.07702	-1.26752
D15	2.84070	.01607	.06729	.00215	.06944	2.91014
D16	-.74808	-.01692	-.07067	-.00257	-.07323	-.82131
D17	-2.84070	-.01607	-.06729	-.00215	-.06944	-2.91014
D18	1.34454	-.01778	-.07405	-.00298	-.07702	1.26752
D19	3.14159	.00000	.00002	.00000	.00000	3.14159
D20	-1.04897	-.00085	-.00336	-.00041	-.00379	-1.05276
D21	1.04897	.00085	.00340	.00041	.00379	1.05276
D22	.74808	.01692	.07067	.00257	.07323	.82131
D23	2.84070	.01607	.06729	.00215	.06944	2.91014
D24	-1.34454	.01778	.07405	.00298	.07702	-1.26752
D25	-.74808	-.01692	-.07067	-.00257	-.07323	-.82131
D26	1.34454	-.01778	-.07405	-.00298	-.07702	1.26752
D27	-2.84070	-.01607	-.06729	-.00215	-.06944	-2.91014

Item	Value	Threshold	Converged?
Maximum Force	.033020	.000450	NO
RMS Force	.014820	.000300	NO
Maximum Displacement	.118834	.001800	NO
RMS Displacement	.044434	.001200	NO

Predicted change in Energy=-8.690843D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	.000000	.000000	-2.358937
2	7	.000000	.000000	-1.175176
3	6	.000000	.000000	.246157
4	6	1.455274	.000019	.753275
5	6	-.727620	-1.260313	.753275

6	6	-.727653	1.260294	.753275
7	1	1.489216	.000019	1.840805
8	1	2.021710	.765127	.196645
9	1	2.021730	-.765075	.196645
10	1	-.744591	-1.289709	1.840805
11	1	-.348236	-2.133416	.196645
12	1	-1.673439	-1.368333	.196645
13	1	-.744625	1.289689	1.840805
14	1	-1.673475	1.368289	.196645
15	1	-.348291	2.133407	.196645

Distance matrix (angstroms):

		1	2	3	4	5
1	C	.000000				
2	N	1.183761	.000000			
3	C	2.605094	1.421333	.000000		
4	C	3.435649	2.415936	1.541100	.000000	
5	C	3.435649	2.415936	1.541100	2.520608	.000000
6	C	3.435649	2.415936	1.541100	2.520608	2.520608
7	H	4.455962	3.363615	2.181895	1.088060	2.772278
8	H	3.347197	2.560200	2.162217	1.102759	3.459923
9	H	3.347197	2.560200	2.162217	1.102759	2.848513
10	H	4.455962	3.363615	2.181895	2.772278	1.088060
11	H	3.347197	2.560200	2.162217	2.848513	1.102759
12	H	3.347197	2.560200	2.162217	3.459923	1.102759
13	H	4.455962	3.363615	2.181895	2.772278	2.772278
14	H	3.347197	2.560200	2.162217	3.459923	2.848513
15	H	3.347197	2.560200	2.162217	2.848513	3.459923

		6	7	8	9	10
6	C	.000000				
7	H	2.772278	.000000			
8	H	2.848513	1.890028	.000000		
9	H	3.459923	1.890028	1.530202	.000000	
10	H	2.772278	2.579398	3.818120	3.260527	.000000
11	H	3.459923	3.260527	3.744088	2.736621	1.890028
12	H	2.848513	3.818120	4.266823	3.744088	1.890028
13	H	1.088060	2.579398	3.260527	3.818120	2.579398
14	H	1.102759	3.818120	3.744088	4.266823	3.260527
15	H	1.102759	3.260527	2.736621	3.744088	3.818120

		11	12	13	14	15
11	H	.000000				
12	H	1.530202	.000000			
13	H	3.818120	3.260527	.000000		
14	H	3.744088	2.736621	1.890028	.000000	
15	H	4.266823	3.744088	1.890028	1.530202	.000000

Stoichiometry C5H9N
Framework group C3V[C3(CNC),3SGV(CH),X(H6)]
Deg. of freedom 9
Full point group C3V NOp 6
Largest Abelian subgroup CS NOp 2
Largest concise Abelian subgroup CS NOp 2

Standard orientation:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	.000000	.000000	2.344987

2	7	.000000	.000000	1.161227
3	6	.000000	.000000	-.260107
4	6	.000000	1.455274	-.767224
5	6	-1.260304	-.727637	-.767224
6	6	1.260304	-.727637	-.767224
7	1	.000000	1.489216	-1.854755
8	1	.765101	2.021720	-.210594
9	1	-.765101	2.021720	-.210594
10	1	-1.289699	-.744608	-1.854755
11	1	-2.133412	-.348263	-.210594
12	1	-1.368311	-1.673457	-.210594
13	1	1.289699	-.744608	-1.854755
14	1	1.368311	-1.673457	-.210594
15	1	2.133412	-.348263	-.210594

```
Rotational constants (GHZ):      4.5446652      2.9282014      2.9282014
Isotopes: C-12,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
Standard basis: 6-31+G(d) (6D, 7F)
There are    85 symmetry adapted basis functions of A'  symmetry.
There are    47 symmetry adapted basis functions of A"  symmetry.
Crude estimate of integral set expansion from redundant integrals=1.123.
Integral buffers will be    262144 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
  132 basis functions      228 primitive gaussians
   23 alpha electrons       23 beta electrons
      nuclear repulsion energy       230.7401687822 Hartrees.
One-electron integrals computed using PRISM.
The smallest eigenvalue of the overlap matrix is  2.672D-05
Initial guess read from the read-write file:
Initial guess orbital symmetries:
      Occupied  (A1) (A1) (A1) (E) (E) (A1) (A1) (A1) (?A) (?A)
                (A1) (?A) (E) (E) (E) (E) (A1) (E) (E) (?A) (?B)
                (?B) (A1)
      Virtual   (A1) (E) (E) (A1) (E) (E) (?A) (?C) (?C) (E) (E)
                (A1) (?D) (?D) (A2) (E) (E) (?A) (A1) (E) (E)
                (A1) (?A) (?E) (?E) (?A) (E) (E) (?F) (?G) (?G)
                (E) (E) (A1) (A1) (E) (E) (?A) (A1) (A1) (E) (E)
                (A1) (E) (E) (?H) (?H) (?A) (E) (E) (?A) (E) (E)
                (A1) (?H) (A1) (E) (E) (E) (E) (?A) (E) (E) (?A)
                (E) (E) (?A) (?E) (?G) (A1) (?C) (?G) (A1) (?F)
                (?H) (A1) (?B) (?E) (?D) (?A) (?A) (?H) (?H) (?H)
                (?F) (?H) (?H) (?D) (?B) (?B) (?B) (?A) (?D) (?H)
                (?B) (?B) (?E) (?H) (?A) (?A) (?C) (?C) (A1) (A1)
                (?C) (?G) (A1) (A1) (?H)
Requested convergence on RMS density matrix=1.00D-08 within  64 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Integral accuracy reduced to 1.0D-05 until final iterations.
Initial convergence to 1.0D-05 achieved.  Increase integral accuracy.
SCF Done:  E(RB-LYP) =  -250.503609571     A.U. after   14 cycles
           Convg  =     .1243D-08             -V/T =  2.0094
           S**2   =    .0000
***** Axes restored to original set *****
-------------------------------------------------------------------
Center     Atomic                     Forces (Hartrees/Bohr)
Number     Number              X              Y              Z
-------------------------------------------------------------------
```

1	6	.000000000	.000000000	-.008550057
2	7	.000000000	.000000000	-.006797619
3	6	.000000000	.000000000	.021311244
4	6	.013101969	.000000171	-.044995102
5	6	-.006550837	-.011346723	-.044995102
6	6	-.006551132	.011346553	-.044995102
7	1	.010353480	.000000135	.003164584
8	1	-.005293697	.026053384	.019921331
9	1	-.005293019	-.026053521	.019921331
10	1	-.005176623	-.008966445	.003164584
11	1	.025209741	-.008442216	.019921331
12	1	-.019916502	.017610649	.019921331
13	1	-.005176857	.008966310	.003164584
14	1	-.019916043	-.017611168	.019921331
15	1	.025209521	.008442872	.019921331

Cartesian Forces: Max .044995102 RMS .017723643
Internal Forces: Max .021998147 RMS .009449354

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Search for a local minimum.
Step number 3 out of a maximum of 77
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Update second derivatives using information from points 2 3
Maximum step size (.424) exceeded in linear search.
-- Step size scaled by .429
-- Skip Quadratic or steepest descent search.
Quartic linear search produced a step of .99388.
Steepest descent instead of Quadratic search.
Iteration 1 RMS(Cart)= .04216055 RMS(Int)= .00162080
Iteration 2 RMS(Cart)= .00142126 RMS(Int)= .00032999
Iteration 3 RMS(Cart)= .00010454 RMS(Int)= .00030526
Iteration 4 RMS(Cart)= .00000697 RMS(Int)= .00030510
TrRot= .000000 .000000 .000000 .000000 .000000 .000000

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.23698	.00855	.00224	.00186	.00410	2.24109
R2	2.68593	.01535	.02995	-.00686	.02309	2.70902
R3	2.91226	.01150	.03903	-.00923	.02980	2.94206
R4	2.91226	.01150	.03903	-.00923	.02980	2.94206
R5	2.91226	.01150	.03903	-.00923	.02980	2.94206
R6	2.05614	.00349	.00868	-.00048	.00820	2.06434
R7	2.08391	.00530	.01964	-.00838	.01126	2.09517
R8	2.08391	.00530	.01964	-.00838	.01126	2.09517
R9	2.05614	.00349	.00868	-.00048	.00820	2.06434
R10	2.08391	.00530	.01964	-.00838	.01126	2.09517
R11	2.08391	.00530	.01964	-.00838	.01126	2.09517
R12	2.05614	.00349	.00868	-.00048	.00820	2.06434
R13	2.08391	.00530	.01964	-.00838	.01126	2.09517
R14	2.08391	.00530	.01964	-.00838	.01126	2.09517
A1	3.14159	.00000	.00000	.00000	.00000	3.14159
A2	3.14159	.00000	.00000	.00000	.00000	3.14159
A3	1.90611	-.00066	-.00306	-.00033	-.00338	1.90272
A4	1.90611	-.00066	-.00306	-.00033	-.00338	1.90272
A5	1.91514	.00066	.00304	.00033	.00334	1.91848
A6	1.90611	-.00066	-.00306	-.00033	-.00338	1.90272

A7	1.91514	.00066	.00304	.00033	.00334	1.91848
A8	1.91514	.00066	.00304	.00033	.00334	1.91848
A9	1.93731	.00625	.01489	-.00184	.01237	1.94967
A10	1.89543	-.00076	-.00826	.00344	-.00537	1.89006
A11	2.08116	-.01222	-.05717	-.00215	-.05988	2.02127
A12	1.89543	-.00076	-.00826	.00344	-.00537	1.89006
A13	2.08116	-.01222	-.05717	-.00215	-.05988	2.02127
A14	1.53352	.02200	.13618	.00013	.13572	1.66924
A15	1.93731	.00625	.01489	-.00184	.01237	1.94967
A16	1.89543	-.00076	-.00826	.00344	-.00537	1.89006
A17	2.08116	-.01222	-.05717	-.00215	-.05988	2.02127
A18	1.89543	-.00076	-.00826	.00344	-.00537	1.89006
A19	2.08116	-.01222	-.05717	-.00215	-.05988	2.02127
A20	1.53352	.02200	.13618	.00013	.13572	1.66924
A21	1.93731	.00625	.01489	-.00184	.01237	1.94967
A22	1.89543	-.00076	-.00826	.00344	-.00537	1.89006
A23	2.08116	-.01222	-.05717	-.00215	-.05988	2.02127
A24	1.89543	-.00076	-.00826	.00344	-.00537	1.89006
A25	2.08116	-.01222	-.05717	-.00215	-.05988	2.02127
A26	1.53352	.02200	.13618	.00013	.13572	1.66924
D1	3.14159	.00000	.00000	.00000	.00000	3.14159
D2	-1.05276	-.00082	-.00377	-.00042	-.00419	-1.05695
D3	1.05276	.00082	.00377	.00042	.00419	1.05695
D4	.82131	.01199	.07278	.00130	.07412	.89544
D5	2.91014	.01118	.06902	.00089	.06993	2.98008
D6	-1.26752	.01281	.07655	.00172	.07832	-1.18920
D7	-.82131	-.01199	-.07278	-.00130	-.07412	-.89544
D8	1.26752	-.01281	-.07655	-.00172	-.07832	1.18920
D9	-2.91014	-.01118	-.06902	-.00089	-.06993	-2.98008
D10	3.14159	.00000	.00000	.00000	.00000	3.14159
D11	1.05276	.00082	.00377	.00042	.00419	1.05695
D12	-1.05276	-.00082	-.00377	-.00042	-.00419	-1.05695
D13	.82131	.01199	.07278	.00130	.07412	.89544
D14	-1.26752	.01281	.07655	.00172	.07832	-1.18920
D15	2.91014	.01118	.06902	.00089	.06993	2.98008
D16	-.82131	-.01199	-.07278	-.00130	-.07412	-.89544
D17	-2.91014	-.01118	-.06902	-.00089	-.06993	-2.98008
D18	1.26752	-.01281	-.07655	-.00172	-.07832	1.18920
D19	3.14159	.00000	.00000	.00000	.00000	3.14159
D20	-1.05276	-.00082	-.00377	-.00042	-.00419	-1.05695
D21	1.05276	.00082	.00377	.00042	.00419	1.05695
D22	.82131	.01199	.07278	.00130	.07412	.89544
D23	2.91014	.01118	.06902	.00089	.06993	2.98008
D24	-1.26752	.01281	.07655	.00172	.07832	-1.18920
D25	-.82131	-.01199	-.07278	-.00130	-.07412	-.89544
D26	1.26752	-.01281	-.07655	-.00172	-.07832	1.18920
D27	-2.91014	-.01118	-.06902	-.00089	-.06993	-2.98008

Item		Value	Threshold	Converged?
Maximum	Force	.021998	.000450	NO
RMS	Force	.009449	.000300	NO
Maximum	Displacement	.106780	.001800	NO
RMS	Displacement	.041897	.001200	NO

Predicted change in Energy=-7.187863D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	.000000	.000000	-2.377638
2	7	.000000	.000000	-1.191706
3	6	.000000	.000000	.241847
4	6	1.471890	.000019	.749174
5	6	-.735928	-1.274703	.749174
6	6	-.735961	1.274684	.749174
7	1	1.523160	.000020	1.840371
8	1	2.015331	.821633	.240376
9	1	2.015352	-.821580	.240376
10	1	-.761563	-1.319105	1.840371
11	1	-.296111	-2.156144	.240376
12	1	-1.719185	-1.334556	.240376
13	1	-.761597	1.319085	1.840371
14	1	-1.719220	1.334511	.240376
15	1	-.296167	2.156136	.240376

Distance matrix (angstroms):

		1	2	3	4	5
1	C	.000000				
2	N	1.185932	.000000			
3	C	2.619485	1.433553	.000000		
4	C	3.455924	2.435872	1.556869	.000000	
5	C	3.455924	2.435872	1.556869	2.549388	.000000
6	C	3.455924	2.435872	1.556869	2.549388	2.549388
7	H	4.484597	3.393155	2.208007	1.092400	2.814091
8	H	3.404502	2.605282	2.176382	1.108716	3.496130
9	H	3.404502	2.605282	2.176382	1.108716	2.834385
10	H	4.484597	3.393155	2.208007	2.814091	1.092400
11	H	3.404502	2.605282	2.176382	2.834385	1.108716
12	H	3.404502	2.605282	2.176382	3.496130	1.108716
13	H	4.484597	3.393155	2.208007	2.814091	2.814091
14	H	3.404502	2.605282	2.176382	3.496130	2.834385
15	H	3.404502	2.605282	2.176382	2.834385	3.496130

		6	7	8	9	10
6	C	.000000				
7	H	2.814091	.000000			
8	H	2.834385	1.864742	.000000		
9	H	3.496130	1.864742	1.643213	.000000	
10	H	2.814091	2.638191	3.854073	3.243265	.000000
11	H	3.496130	3.243265	3.769604	2.669067	1.864742
12	H	2.834385	3.854073	4.312280	3.769604	1.864742
13	H	1.092400	2.638191	3.243265	3.854073	2.638191
14	H	1.108716	3.854073	3.769604	4.312280	3.243265
15	H	1.108716	3.243265	2.669067	3.769604	3.854073

		11	12	13	14	15
11	H	.000000				
12	H	1.643213	.000000			
13	H	3.854073	3.243265	.000000		
14	H	3.769604	2.669067	1.864742	.000000	
15	H	4.312280	3.769604	1.864742	1.643213	.000000

Stoichiometry C5H9N
Framework group C3V[C3(CNC),3SGV(CH),X(H6)]
Deg. of freedom 9
Full point group C3V NOp 6

```
Largest Abelian subgroup         CS      NOp   2
Largest concise Abelian subgroup CS      NOp   2
                  Standard orientation:
---------------------------------------------------------------------
Center     Atomic                 Coordinates (Angstroms)
Number     Number              X           Y           Z
---------------------------------------------------------------------
   1          6             .000000     .000000    2.362243
   2          7             .000000     .000000    1.176310
   3          6             .000000     .000000    -.257242
   4          6             .000000    1.471890    -.764569
   5          6           -1.274694    -.735945    -.764569
   6          6            1.274694    -.735945    -.764569
   7          1             .000000    1.523160   -1.855766
   8          1             .821606    2.015341    -.255772
   9          1            -.821606    2.015341    -.255772
  10          1           -1.319095    -.761580   -1.855766
  11          1           -2.156140    -.296139    -.255772
  12          1           -1.334534   -1.719203    -.255772
  13          1            1.319095    -.761580   -1.855766
  14          1            1.334534   -1.719203    -.255772
  15          1            2.156140    -.296139    -.255772
---------------------------------------------------------------------
Rotational constants (GHZ):      4.4468315      2.8843982      2.8843982
Isotopes: C-12,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
Standard basis: 6-31+G(d) (6D, 7F)
There are    85 symmetry adapted basis functions of A'  symmetry.
There are    47 symmetry adapted basis functions of A"  symmetry.
Crude estimate of integral set expansion from redundant integrals=1.123.
Integral buffers will be    262144 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
  132 basis functions      228 primitive gaussians
   23 alpha electrons       23 beta electrons
      nuclear repulsion energy       228.8666497423 Hartrees.
One-electron integrals computed using PRISM.
The smallest eigenvalue of the overlap matrix is  2.751D-05
Initial guess read from the read-write file:
Initial guess orbital symmetries:
      Occupied  (A1) (A1) (A1) (E) (E) (A1) (A1) (A1) (?A) (?A)
                (A1) (?A) (E) (E) (E) (E) (A1) (?B) (?B) (?A)
                (?C) (?C) (A1)
      Virtual   (A1) (E) (E) (A1) (E) (E) (?A) (?D) (?D) (E) (E)
                (A1) (?E) (?E) (A2) (?A) (E) (E) (A1) (E) (E)
                (A1) (?A) (?F) (?F) (?A) (?C) (?C) (E) (E) (E)
                (E) (E) (A1) (A1) (E) (E) (A1) (A1) (A1) (E) (E)
                (A1) (E) (E) (?A) (?G) (?G) (E) (E) (?A) (E) (E)
                (A1) (A1) (?G) (E) (E) (E) (E) (?A) (E) (E) (?A)
                (E) (E) (A1) (A1) (?F) (?F) (?D) (?C) (A1) (?F)
                (?F) (A1) (E) (?F) (?E) (?A) (?A) (A1) (E) (?G)
                (?F) (?G) (?G) (?E) (?B) (?B) (?C) (?A) (?E) (A1)
                (?B) (?C) (?F) (?G) (?A) (?A) (?D) (?D) (A1) (A1)
                (A1) (?D) (?C) (A1) (?G)
Requested convergence on RMS density matrix=1.00D-08 within  64 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Integral accuracy reduced to 1.0D-05 until final iterations.
Initial convergence to 1.0D-05 achieved.  Increase integral accuracy.
```

```
SCF Done:  E(RB-LYP) =  -250.528455256     A.U. after   12 cycles
            Convg  =     .8627D-08             -V/T =  2.0102
            S**2   =    .0000
***** Axes restored to original set *****
-------------------------------------------------------------------
Center     Atomic                   Forces (Hartrees/Bohr)
Number     Number              X              Y              Z
-------------------------------------------------------------------
   1          6           .000000000     .000000000    -.004493326
   2          7           .000000000     .000000000    -.002036641
   3          6           .000000000     .000000000     .023620505
   4          6           .007906600     .000000103    -.038753680
   5          6          -.003953211    -.006847368    -.038753680
   6          6          -.003953389     .006847265    -.038753680
   7          1           .005314513     .000000069     .001723817
   8          1          -.004423382     .011487495     .015666508
   9          1          -.004423083    -.011487610     .015666508
  10          1          -.002657197    -.004602538     .001723817
  11          1           .012160153    -.001912986     .015666508
  12          1          -.007737021     .009574307     .015666508
  13          1          -.002657316     .004602469     .001723817
  14          1          -.007736771    -.009574508     .015666508
  15          1           .012160103     .001913303     .015666508
-------------------------------------------------------------------
Cartesian Forces:  Max      .038753680 RMS      .013124031
Internal  Forces:  Max      .011879111 RMS      .005466971

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Search for a local minimum.
Step number   4 out of a maximum of  77
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Update second derivatives using information from points  3  4
Maximum step size (    .424) exceeded in linear search.
   -- Step size scaled by    .649
   -- Skip Quadratic or steepest descent search.
Quartic linear search produced a step of   .99760.
Steepest descent instead of Quadratic search.
Iteration  1 RMS(Cart)=   .04041277 RMS(Int)=   .00163700
Iteration  2 RMS(Cart)=   .00146266 RMS(Int)=   .00040073
Iteration  3 RMS(Cart)=   .00010302 RMS(Int)=   .00037954
Iteration  4 RMS(Cart)=   .00000719 RMS(Int)=   .00037939
TrRot=   .000000   .000000   .000000   .000000   .000000   .000000
Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                                 (Linear)    (Quad)   (Total)
   R1         2.24109    .00449    .00409   -.00085    .00324   2.24433
   R2         2.70902    .00653    .02304   -.00339    .01965   2.72867
   R3         2.94206    .00228    .02973   -.00578    .02394   2.96600
   R4         2.94206    .00228    .02973   -.00578    .02394   2.96600
   R5         2.94206    .00228    .02973   -.00578    .02394   2.96600
   R6         2.06434    .00197    .00818   -.00013    .00805   2.07239
   R7         2.09517   -.00084    .01123   -.00509    .00614   2.10131
   R8         2.09517   -.00084    .01123   -.00509    .00614   2.10131
   R9         2.06434    .00197    .00818   -.00013    .00805   2.07239
  R10         2.09517   -.00084    .01123   -.00509    .00614   2.10131
  R11         2.09517   -.00084    .01123   -.00509    .00614   2.10131
  R12         2.06434    .00197    .00818   -.00013    .00805   2.07239
```