**Mechanistic formation of hazardous molecular heterocyclic amines from high temperature pyrolysis of model biomass materials: cellulose and tyrosine**

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**Additional Supporting Information**

**S1. Tar and Char Data**

|  |  |
| --- | --- |
| Temp. ($°C)$ | % Yield |
| Tar | Error Tar | Temp. 2 | Char | Error Char |
| 200 | 1.34 | 0.6 | 200 | 95.2 | 2.9 |
| 250 | 1.79 | 0.8 | 300 | 78.8 | 3.3 |
| 300 | 5.68 | 0.95 | 350 | 53.5 | 3.1 |
| 350 | 10.75 | 1.1 | 400 | 30.1 | 2.4 |
| 400 | 21.29 | 1.4 | 450 | 26.6 | 3.2 |
| 450 | 33.04 | 1.5 | 500 | 26.3 | 2.9 |
| 500 | 22.32 | 1.6 | 600 | 24 | 2.8 |
| 550 | 14.29 | 1.15 | 700 | 19.2 | 2.2 |
| 600 | 6.82 | 1.12 |  |  |  |
| 650 | 4.36 | 1.1 |  |  |  |
| 700 | 2.68 | 0.8 |  |  |  |
| 750 | 1.79 | 0.2 |  |  |  |

**S2: % Yields of Tar and Char**

|  |  |  |
| --- | --- | --- |
| Temp. ($°C)$ | Conc. (ug) | % Yield |
| isoindazole | Error | 1-methyl indazole | Error | 1-naphthyl isocyanate | Error | Char Yield | Error |
| 200 | 10.55 | 1.5 | 0.64 | 0.2 | 5.05 | 1.3 | 95.2 | 2.9 |
| 300 | 127 | 4.1 | 252 | 8.8 | 19.7 | 3.2 | 78.8 | 3.3 |
| 350 | 163 | 8.2 | 29.15 | 3.1 | 119.5 | 8.5 | 53.5 | 3.1 |
| 400 | 183 | 10.8 | 9.8 | 1.8 | 110 | 7.8 | 30.1 | 2.4 |
| 450 | 130 | 6.3 | 4.87 | 1.2 | 51.5 | 5.92 | 26.6 | 3.2 |
| 500 | 56 | 3.1 | 1.74 | 0.92 | 18.8 | 2.91 | 26.3 | 2.9 |
| 600 | 34 | 2.6 | 0.63 | 0.15 | 6.1 | 1.45 | 24 | 2.8 |
| 700 | 27.65 | 1.25 | 0.161 | 0.4 | 4.885 | 0.8 | 19.2 | 2.2 |

**S3: Input and Optimized molecular structures of compounds of interest**



Input structure for Isoindazole



Optimized structure for isoindazole



Input structure for 1-methyl indole



Optimized structure for 1-methyl indole



Input structure of 1-naphthylisocyanate



Optimized structure of 1-naphthylisocyanate

**S4: Molecular orbital diagrams for compounds of interest**



1-naphthylisocyanate



Isoindazole



1-methylindazole

**S5: Example of optimization Energies**

1. **Isoindole**

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 - Thermochemistry -

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 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 6 and mass 12.00000

 Atom 7 has atomic number 6 and mass 12.00000

 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 7 and mass 14.00307

 Atom 15 has atomic number 7 and mass 14.00307

 Molecular mass: 118.05310 amu.

 Principal axes and moments of inertia in atomic units:

 1 2 3

 EIGENVALUES -- 457.164021116.971451574.13544

 X 1.00000 0.00161 0.00000

 Y -0.00161 1.00000 -0.00001

 Z 0.00000 0.00001 1.00000

 This molecule is an asymmetric top.

 Rotational symmetry number 1.

 Warning -- assumption of classical behavior for rotation

 may cause significant error

 Rotational temperatures (Kelvin) 0.18946 0.07754 0.05502

 Rotational constants (GHZ): 3.94769 1.61575 1.14650

 Zero-point vibrational energy 312160.9 (Joules/Mol)

 74.60825 (Kcal/Mol)

 Warning -- explicit consideration of 7 degrees of freedom as

 vibrations may cause significant error

 Vibrational temperatures: 319.19 377.35 584.79 649.03 771.32

 (Kelvin) 803.65 865.32 929.17 951.91 1115.15

 1120.61 1173.73 1263.03 1321.61 1331.39

 1343.84 1415.24 1452.64 1476.61 1498.61

 1679.11 1740.06 1782.01 1840.13 1857.39

 1885.13 1981.70 2034.73 2048.67 2183.23

 2215.54 2305.24 2373.00 4596.21 4607.50

 4623.56 4637.89 4718.16 5215.13

 Zero-point correction= 0.118896 (Hartree/Particle)

 Thermal correction to Energy= 0.124809

 Thermal correction to Enthalpy= 0.125753

 Thermal correction to Gibbs Free Energy= 0.088779

 Sum of electronic and zero-point Energies= -377.623299

 Sum of electronic and thermal Energies= -377.617386

 Sum of electronic and thermal Enthalpies= -377.616441

 Sum of electronic and thermal Free Energies= -377.653415

 E (Thermal) CV S

 KCal/Mol Cal/Mol-Kelvin Cal/Mol-Kelvin

 Total 78.319 24.470 77.818

 Electronic 0.000 0.000 0.000

 Translational 0.889 2.981 40.213

 Rotational 0.889 2.981 28.177

 Vibrational 76.541 18.509 9.429

 Vibration 1 0.648 1.808 1.944

 Vibration 2 0.670 1.742 1.647

 Vibration 3 0.771 1.456 0.939

 Vibration 4 0.810 1.358 0.792

 Vibration 5 0.891 1.170 0.574

 Vibration 6 0.914 1.121 0.527

 Vibration 7 0.960 1.029 0.447

 Q Log10(Q) Ln(Q)

 Total Bot 0.146023D-40 -40.835579 -94.027396

 Total V=0 0.712173D+14 13.852585 31.896757

 Vib (Bot) 0.902454D-54 -54.044575 -124.442233

 Vib (Bot) 1 0.890927D+00 -0.050158 -0.115492

 Vib (Bot) 2 0.739750D+00 -0.130915 -0.301443

 Vib (Bot) 3 0.436438D+00 -0.360078 -0.829110

 Vib (Bot) 4 0.379817D+00 -0.420425 -0.968065

 Vib (Bot) 5 0.296628D+00 -0.527788 -1.215276

 Vib (Bot) 6 0.278644D+00 -0.554951 -1.277822

 Vib (Bot) 7 0.247910D+00 -0.605706 -1.394690

 Vib (V=0) 0.440139D+01 0.643590 1.481920

 Vib (V=0) 1 0.152164D+01 0.182312 0.419790

 Vib (V=0) 2 0.139288D+01 0.143913 0.331372

 Vib (V=0) 3 0.116368D+01 0.065835 0.151592

 Vib (V=0) 4 0.112790D+01 0.052271 0.120359

 Vib (V=0) 5 0.108137D+01 0.033973 0.078227

 Vib (V=0) 6 0.107240D+01 0.030357 0.069900

 Vib (V=0) 7 0.105809D+01 0.024521 0.056461

 Electronic 0.100000D+01 0.000000 0.000000

 Translational 0.504163D+08 7.702571 17.735826

 Rotational 0.320940D+06 5.506424 12.679011

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

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 Center Atomic Forces (Hartrees/Bohr)

 Number Number X Y Z

 -------------------------------------------------------------------

 1 6 -0.000092853 -0.000025933 0.000085968

 2 6 -0.000037442 -0.000147501 -0.000086134

 3 6 -0.000000889 0.000027959 -0.000045994

 4 6 -0.000030606 -0.000006079 0.000016402

 5 6 0.000022403 0.000002201 0.000014662

 6 6 -0.000005426 -0.000006847 -0.000013920

 7 6 -0.000038162 -0.000054237 0.000140762

 8 1 0.000010668 0.000000195 0.000010953

 9 1 0.000004940 0.000009089 0.000000525

 10 1 -0.000005361 0.000007416 -0.000005159

 11 1 -0.000010566 0.000009105 -0.000000866

 12 1 0.000044378 0.000047200 -0.000010898

 13 1 0.000000693 -0.000011559 -0.000019510

 14 7 0.000102761 0.000120959 -0.000078188

 15 7 0.000035463 0.000028034 -0.000008603

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 Cartesian Forces: Max 0.000147501 RMS 0.000050664

 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

 Berny optimization.

 Internal Forces: Max 0.000137168 RMS 0.000029317

 Search for a local minimum.

 Step number 1 out of a maximum of 2

 All quantities printed in internal units (Hartrees-Bohrs-Radians)

 Second derivative matrix not updated -- analytic derivatives used.

 Eigenvalues --- 0.00707 0.01188 0.01734 0.01759 0.01985

 Eigenvalues --- 0.02178 0.02410 0.02567 0.03163 0.03234

 Eigenvalues --- 0.04132 0.05556 0.10799 0.11286 0.11577

 Eigenvalues --- 0.11868 0.12991 0.13234 0.16730 0.19700

 Eigenvalues --- 0.20292 0.20814 0.23710 0.25790 0.30039

 Eigenvalues --- 0.34632 0.35931 0.36266 0.36502 0.36624

 Eigenvalues --- 0.37781 0.38677 0.39997 0.40238 0.45619

 Eigenvalues --- 0.46906 0.47430 0.50225 0.512801000.00000

 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 --- 1000.000001000.00000

 Angle between quadratic step and forces= 56.07 degrees.

 Linear search not attempted -- first point.

 Iteration 1 RMS(Cart)= 0.00018610 RMS(Int)= 0.00000006

 Iteration 2 RMS(Cart)= 0.00000005 RMS(Int)= 0.00000005

 Variable Old X -DE/DX Delta X Delta X Delta X New X

 (Linear) (Quad) (Total)

 R1 2.69437 0.00003 0.00000 0.00013 0.00013 2.69450

 R2 2.65071 0.00001 0.00000 0.00000 0.00000 2.65071

 R3 2.59237 -0.00012 0.00000 -0.00023 -0.00023 2.59214

 R4 2.65234 0.00003 0.00000 0.00008 0.00008 2.65242

 R5 2.70823 -0.00003 0.00000 -0.00009 -0.00009 2.70814

 R6 2.62056 0.00001 0.00000 0.00002 0.00002 2.62058

 R7 2.04801 0.00001 0.00000 0.00003 0.00003 2.04804

 R8 2.67335 -0.00002 0.00000 -0.00006 -0.00006 2.67329

 R9 2.04717 0.00001 0.00000 0.00003 0.00003 2.04721

 R10 2.62177 0.00000 0.00000 0.00001 0.00001 2.62178

 R11 2.04819 0.00001 0.00000 0.00002 0.00002 2.04821

 R12 2.04654 0.00001 0.00000 0.00003 0.00003 2.04657

 R13 2.03578 0.00001 0.00000 0.00002 0.00002 2.03579

 R14 2.52124 -0.00014 0.00000 -0.00025 -0.00025 2.52098

 R15 1.90755 -0.00006 0.00000 -0.00012 -0.00012 1.90743

 R16 2.66669 0.00000 0.00000 -0.00009 -0.00009 2.66660

 A1 2.11548 0.00003 0.00000 0.00009 0.00009 2.11557

 A2 1.85204 -0.00006 0.00000 -0.00016 -0.00016 1.85188

 A3 2.31566 0.00002 0.00000 0.00008 0.00008 2.31574

 A4 2.09462 -0.00004 0.00000 -0.00015 -0.00015 2.09448

 A5 1.83019 0.00004 0.00000 0.00011 0.00011 1.83030

 A6 2.35837 0.00000 0.00000 0.00004 0.00004 2.35841

 A7 2.06974 0.00001 0.00000 0.00004 0.00004 2.06978

 A8 2.10369 0.00000 0.00000 0.00000 0.00000 2.10369

 A9 2.10975 0.00000 0.00000 -0.00003 -0.00003 2.10972

 A10 2.11043 0.00002 0.00000 0.00005 0.00005 2.11048

 A11 2.09366 -0.00001 0.00000 -0.00004 -0.00004 2.09362

 A12 2.07909 -0.00001 0.00000 -0.00002 -0.00002 2.07908

 A13 2.12275 0.00000 0.00000 -0.00002 -0.00002 2.12273

 A14 2.07882 0.00000 0.00000 0.00002 0.00002 2.07884

 A15 2.08161 0.00000 0.00000 0.00000 0.00000 2.08161

 A16 2.05335 -0.00001 0.00000 -0.00002 -0.00002 2.05334

 A17 2.11952 0.00001 0.00000 0.00006 0.00006 2.11958

 A18 2.11031 0.00000 0.00000 -0.00005 -0.00005 2.11026

 A19 2.23012 0.00003 0.00000 0.00012 0.00012 2.23024

 A20 1.95857 -0.00005 0.00000 -0.00013 -0.00013 1.95844

 A21 2.09450 0.00002 0.00000 0.00001 0.00001 2.09451

 A22 1.82861 0.00005 0.00000 0.00011 0.00011 1.82872

 A23 2.26004 -0.00004 0.00000 -0.00027 -0.00027 2.25976

 A24 1.95537 0.00002 0.00000 0.00007 0.00007 1.95544

 A25 2.06778 0.00002 0.00000 0.00020 0.00020 2.06798

 D1 -0.00010 0.00000 0.00000 0.00010 0.00010 0.00000

 D2 -3.14134 -0.00001 0.00000 -0.00025 -0.00025 3.14159

 D3 -3.14132 -0.00002 0.00000 -0.00027 -0.00027 -3.14159

 D4 0.00062 -0.00003 0.00000 -0.00062 -0.00062 0.00000

 D5 0.00026 -0.00001 0.00000 -0.00026 -0.00026 0.00000

 D6 -3.14137 -0.00001 0.00000 -0.00022 -0.00022 3.14159

 D7 3.14137 0.00001 0.00000 0.00022 0.00022 3.14159

 D8 -0.00026 0.00001 0.00000 0.00026 0.00026 0.00000

 D9 3.14104 0.00002 0.00000 0.00056 0.00056 -3.14159

 D10 -0.00024 0.00001 0.00000 0.00024 0.00024 0.00000

 D11 -0.00012 0.00000 0.00000 0.00012 0.00012 0.00000

 D12 -3.14140 -0.00001 0.00000 -0.00020 -0.00020 3.14159

 D13 -0.00013 0.00001 0.00000 0.00013 0.00013 0.00000

 D14 -3.14126 -0.00001 0.00000 -0.00033 -0.00033 3.14159

 D15 3.14098 0.00002 0.00000 0.00061 0.00061 -3.14159

 D16 -0.00015 0.00001 0.00000 0.00015 0.00015 0.00000

 D17 -3.14122 0.00000 0.00000 -0.00037 -0.00037 3.14159

 D18 -0.00085 0.00004 0.00000 0.00085 0.00085 0.00000

 D19 0.00080 -0.00002 0.00000 -0.00080 -0.00080 0.00000

 D20 3.14117 0.00003 0.00000 0.00042 0.00042 3.14159

 D21 0.00019 -0.00001 0.00000 -0.00019 -0.00019 0.00000

 D22 -3.14146 -0.00001 0.00000 -0.00013 -0.00013 -3.14159

 D23 3.14132 0.00001 0.00000 0.00027 0.00027 -3.14159

 D24 -0.00033 0.00001 0.00000 0.00033 0.00033 0.00000

 D25 -0.00002 0.00000 0.00000 0.00002 0.00002 0.00000

 D26 3.14136 0.00001 0.00000 0.00023 0.00023 -3.14159

 D27 -3.14156 0.00000 0.00000 -0.00003 -0.00003 3.14159

 D28 -0.00018 0.00001 0.00000 0.00018 0.00018 0.00000

 D29 -0.00020 0.00001 0.00000 0.00020 0.00020 0.00000

 D30 3.14143 0.00001 0.00000 0.00016 0.00016 -3.14159

 D31 -3.14158 0.00000 0.00000 -0.00001 -0.00001 3.14159

 D32 0.00005 0.00000 0.00000 -0.00005 -0.00005 0.00000

 D33 0.00070 -0.00004 0.00000 -0.00070 -0.00070 0.00000

 D34 3.14118 0.00001 0.00000 0.00042 0.00042 -3.14159

 D35 -0.00028 0.00002 0.00000 0.00028 0.00028 0.00000

 D36 3.14159 0.00001 0.00000 0.00000 0.00000 3.14159

 Item Value Threshold Converged?

 Maximum Force 0.000137 0.000450 YES

 RMS Force 0.000029 0.000300 YES

 Maximum Displacement 0.000813 0.001800 YES

 RMS Displacement 0.000186 0.001200 YES

 Predicted change in Energy=-1.602428D-07

 Optimization completed.

 -- Stationary point found.

**b) 1-methyl indazole**

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 - Thermochemistry -

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 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 6 and mass 12.00000

 Atom 7 has atomic number 6 and mass 12.00000

 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 7 and mass 14.00307

 Atom 14 has atomic number 7 and mass 14.00307

 Atom 15 has atomic number 6 and mass 12.00000

 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

 Molecular mass: 132.06875 amu.

 Principal axes and moments of inertia in atomic units:

 1 2 3

 EIGENVALUES -- 647.583651394.177462030.52179

 X 0.99922 -0.03950 0.00000

 Y 0.03950 0.99922 0.00000

 Z 0.00000 0.00000 1.00000

 This molecule is an asymmetric top.

 Rotational symmetry number 1.

 Warning -- assumption of classical behavior for rotation

 may cause significant error

 Rotational temperatures (Kelvin) 0.13375 0.06213 0.04266

 Rotational constants (GHZ): 2.78689 1.29448 0.88881

 Zero-point vibrational energy 414007.9 (Joules/Mol)

 98.95026 (Kcal/Mol)

 Warning -- explicit consideration of 8 degrees of freedom as

 vibrations may cause significant error

 Vibrational temperatures: 120.02 218.15 365.83 376.84 458.09

 (Kelvin) 728.70 739.70 840.18 928.81 947.40

 1027.71 1140.63 1197.23 1261.05 1323.56

 1449.05 1457.09 1483.58 1524.72 1580.26

 1635.76 1700.41 1757.27 1796.95 1823.23

 1841.57 1918.54 1941.76 1989.86 2063.17

 2114.65 2173.82 2263.32 2325.28 2357.98

 2396.10 2400.27 2424.84 2495.38 2571.87

 4605.98 4677.49 4783.38 4826.20 4838.57

 4861.87 4875.42 4957.77

 Zero-point correction= 0.157687 (Hartree/Particle)

 Thermal correction to Energy= 0.164826

 Thermal correction to Enthalpy= 0.165770

 Thermal correction to Gibbs Free Energy= 0.125430

 Sum of electronic and zero-point Energies= -413.988195

 Sum of electronic and thermal Energies= -413.981056

 Sum of electronic and thermal Enthalpies= -413.980112

 Sum of electronic and thermal Free Energies= -414.020452

 E (Thermal) CV S

 KCal/Mol Cal/Mol-Kelvin Cal/Mol-Kelvin

 Total 103.430 27.183 84.902

 Electronic 0.000 0.000 0.000

 Translational 0.889 2.981 40.547

 Rotational 0.889 2.981 28.996

 Vibrational 101.652 21.221 15.359

 Vibration 1 0.600 1.961 3.809

 Vibration 2 0.619 1.901 2.652

 Vibration 3 0.665 1.756 1.701

 Vibration 4 0.669 1.743 1.649

 Vibration 5 0.705 1.638 1.318

 Vibration 6 0.862 1.236 0.642

 Vibration 7 0.869 1.219 0.624

 Vibration 8 0.941 1.066 0.478

 Q Log10(Q) Ln(Q)

 Total Bot 0.202388D-57 -57.693816 -132.844920

 Total V=0 0.687298D+15 14.837145 34.163789

 Vib (Bot) 0.699958D-71 -71.154928 -163.840277

 Vib (Bot) 1 0.246752D+01 0.392261 0.903215

 Vib (Bot) 2 0.133673D+01 0.126044 0.290227

 Vib (Bot) 3 0.766034D+00 -0.115752 -0.266529

 Vib (Bot) 4 0.740867D+00 -0.130260 -0.299935

 Vib (Bot) 5 0.590982D+00 -0.228426 -0.525970

 Vib (Bot) 6 0.322638D+00 -0.491285 -1.131225

 Vib (Bot) 7 0.315654D+00 -0.500788 -1.153107

 Vib (Bot) 8 0.259912D+00 -0.585174 -1.347414

 Vib (V=0) 0.237702D+02 1.376033 3.168432

 Vib (V=0) 1 0.301767D+01 0.479672 1.104485

 Vib (V=0) 2 0.192718D+01 0.284923 0.656059

 Vib (V=0) 3 0.141477D+01 0.150686 0.346968

 Vib (V=0) 4 0.139380D+01 0.144201 0.332036

 Vib (V=0) 5 0.127412D+01 0.105210 0.242255

 Vib (V=0) 6 0.109506D+01 0.039438 0.090808

 Vib (V=0) 7 0.109130D+01 0.037945 0.087371

 Vib (V=0) 8 0.106352D+01 0.026745 0.061584

 Electronic 0.100000D+01 0.000000 0.000000

 Translational 0.596562D+08 7.775655 17.904108

 Rotational 0.484682D+06 5.685457 13.091249

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

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 Center Atomic Forces (Hartrees/Bohr)

 Number Number X Y Z

 -------------------------------------------------------------------

 1 6 -0.000038148 -0.000062210 -0.000006627

 2 6 0.000017516 -0.000034242 -0.000010342

 3 6 0.000022241 0.000009021 0.000026979

 4 6 -0.000006401 0.000003300 0.000002165

 5 6 0.000015731 -0.000018517 -0.000031063

 6 6 0.000005627 0.000037546 0.000046580

 7 6 -0.000000789 -0.000001688 -0.000022978

 8 1 -0.000002441 0.000000966 -0.000006960

 9 1 -0.000000048 0.000002668 -0.000002833

 10 1 -0.000000841 0.000002337 0.000001724

 11 1 0.000003355 0.000000631 -0.000005712

 12 1 -0.000004251 -0.000002813 0.000002820

 13 7 -0.000031722 0.000005818 -0.000019778

 14 7 0.000009870 0.000027224 0.000013123

 15 6 0.000012204 0.000030798 0.000013081

 16 1 -0.000006362 0.000004252 -0.000004669

 17 1 -0.000003595 -0.000000685 -0.000001412

 18 1 0.000008055 -0.000004404 0.000005903

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 Cartesian Forces: Max 0.000062210 RMS 0.000018307

 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

 Berny optimization.

 Internal Forces: Max 0.000047495 RMS 0.000011287

 Search for a local minimum.

 Step number 1 out of a maximum of 2

 All quantities printed in internal units (Hartrees-Bohrs-Radians)

 Second derivative matrix not updated -- analytic derivatives used.

 Eigenvalues --- 0.00052 0.00720 0.01452 0.02120 0.02193

 Eigenvalues --- 0.02442 0.02785 0.03051 0.03244 0.03912

 Eigenvalues --- 0.04051 0.04768 0.06250 0.07479 0.07573

 Eigenvalues --- 0.12602 0.13093 0.13572 0.14714 0.14988

 Eigenvalues --- 0.15302 0.16489 0.19651 0.21445 0.21888

 Eigenvalues --- 0.23165 0.23648 0.24943 0.26690 0.27492

 Eigenvalues --- 0.32274 0.36661 0.37271 0.39010 0.39424

 Eigenvalues --- 0.39866 0.40102 0.40278 0.40461 0.41288

 Eigenvalues --- 0.42427 0.43443 0.44857 0.45376 0.53392

 Eigenvalues --- 0.54742 0.57564 0.630851000.000001000.00000

 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

 Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000

 Eigenvalues --- 1000.000001000.00000

 Angle between quadratic step and forces= 51.33 degrees.

 Linear search not attempted -- first point.

 Iteration 1 RMS(Cart)= 0.00017869 RMS(Int)= 0.00000002

 Iteration 2 RMS(Cart)= 0.00000003 RMS(Int)= 0.00000001

 Variable Old X -DE/DX Delta X Delta X Delta X New X

 (Linear) (Quad) (Total)

 R1 2.64297 0.00001 0.00000 0.00005 0.00005 2.64302

 R2 2.63409 0.00003 0.00000 0.00009 0.00009 2.63418

 R3 2.71020 -0.00001 0.00000 -0.00003 -0.00003 2.71016

 R4 2.63930 0.00002 0.00000 0.00005 0.00005 2.63934

 R5 2.56816 -0.00005 0.00000 -0.00010 -0.00010 2.56806

 R6 2.58935 -0.00001 0.00000 -0.00002 -0.00002 2.58932

 R7 2.02347 0.00000 0.00000 -0.00001 -0.00001 2.02346

 R8 2.65964 -0.00001 0.00000 -0.00002 -0.00002 2.65962

 R9 2.02608 0.00000 0.00000 0.00000 0.00000 2.02608

 R10 2.59002 0.00000 0.00000 -0.00002 -0.00002 2.59001

 R11 2.02446 0.00000 0.00000 0.00001 0.00001 2.02447

 R12 2.02610 0.00000 0.00000 -0.00001 -0.00001 2.02610

 R13 2.01281 0.00000 0.00000 0.00001 0.00001 2.01282

 R14 2.45575 -0.00001 0.00000 0.00001 0.00001 2.45576

 R15 2.62656 -0.00001 0.00000 -0.00008 -0.00008 2.62648

 R16 2.74163 -0.00001 0.00000 -0.00003 -0.00003 2.74160

 R17 2.04704 0.00000 0.00000 0.00000 0.00000 2.04704

 R18 2.03693 0.00000 0.00000 0.00001 0.00001 2.03695

 R19 2.04702 0.00001 0.00000 0.00002 0.00002 2.04704

 A1 2.10157 -0.00003 0.00000 -0.00012 -0.00012 2.10144

 A2 1.82348 0.00001 0.00000 0.00001 0.00001 1.82348

 A3 2.35814 0.00002 0.00000 0.00012 0.00012 2.35826

 A4 2.11485 0.00002 0.00000 0.00009 0.00009 2.11494

 A5 1.86911 -0.00001 0.00000 -0.00003 -0.00003 1.86908

 A6 2.29923 -0.00001 0.00000 -0.00006 -0.00006 2.29916

 A7 2.05094 0.00000 0.00000 -0.00002 -0.00002 2.05091

 A8 2.11797 0.00000 0.00000 -0.00001 -0.00001 2.11797

 A9 2.11428 0.00000 0.00000 0.00003 0.00003 2.11430

 A10 2.12479 0.00000 0.00000 -0.00003 -0.00003 2.12476

 A11 2.08266 0.00000 0.00000 0.00003 0.00003 2.08269

 A12 2.07574 0.00000 0.00000 -0.00001 -0.00001 2.07573

 A13 2.10583 0.00001 0.00000 0.00006 0.00006 2.10589

 A14 2.07965 -0.00001 0.00000 -0.00002 -0.00002 2.07963

 A15 2.09771 -0.00001 0.00000 -0.00004 -0.00004 2.09767

 A16 2.06840 0.00000 0.00000 0.00002 0.00002 2.06843

 A17 2.10473 0.00000 0.00000 0.00001 0.00001 2.10473

 A18 2.11005 0.00000 0.00000 -0.00003 -0.00003 2.11002

 A19 2.23120 0.00001 0.00000 0.00005 0.00005 2.23125

 A20 1.94122 -0.00002 0.00000 -0.00004 -0.00004 1.94118

 A21 2.11077 0.00001 0.00000 -0.00001 -0.00001 2.11075

 A22 1.92868 0.00001 0.00000 0.00004 0.00004 1.92872

 A23 2.25824 -0.00004 0.00000 -0.00022 -0.00022 2.25803

 A24 2.09626 0.00003 0.00000 0.00017 0.00017 2.09644

 A25 1.86230 0.00001 0.00000 0.00001 0.00001 1.86231

 A26 1.93411 -0.00001 0.00000 -0.00008 -0.00008 1.93402

 A27 1.86847 0.00000 0.00000 0.00001 0.00001 1.86848

 A28 1.93396 0.00001 0.00000 0.00006 0.00006 1.93402

 A29 1.90949 0.00000 0.00000 -0.00002 -0.00002 1.90947

 A30 1.90783 0.00000 0.00000 0.00003 0.00003 1.90786

 A31 1.90946 0.00000 0.00000 0.00000 0.00000 1.90947

 D1 0.00004 0.00000 0.00000 -0.00004 -0.00004 0.00000

 D2 -3.14152 0.00000 0.00000 -0.00008 -0.00008 3.14159

 D3 -3.14159 0.00000 0.00000 -0.00001 -0.00001 -3.14159

 D4 0.00005 0.00000 0.00000 -0.00005 -0.00005 0.00000

 D5 -0.00030 0.00001 0.00000 0.00030 0.00030 0.00000

 D6 -3.14158 0.00000 0.00000 -0.00001 -0.00001 3.14159

 D7 3.14133 0.00001 0.00000 0.00026 0.00026 3.14159

 D8 0.00005 0.00000 0.00000 -0.00005 -0.00005 0.00000

 D9 -3.14155 0.00000 0.00000 -0.00005 -0.00005 3.14159

 D10 -0.00010 0.00001 0.00000 0.00010 0.00010 0.00000

 D11 0.00001 0.00000 0.00000 -0.00001 -0.00001 0.00000

 D12 3.14146 0.00001 0.00000 0.00013 0.00013 -3.14159

 D13 0.00020 -0.00001 0.00000 -0.00020 -0.00020 0.00000

 D14 3.14154 0.00000 0.00000 0.00005 0.00005 3.14159

 D15 -3.14145 0.00000 0.00000 -0.00014 -0.00014 -3.14159

 D16 -0.00011 0.00001 0.00000 0.00011 0.00011 0.00000

 D17 0.00002 0.00000 0.00000 -0.00002 -0.00002 0.00000

 D18 3.14138 0.00000 0.00000 0.00021 0.00021 -3.14159

 D19 -3.14153 0.00000 0.00000 -0.00006 -0.00006 3.14159

 D20 -0.00016 0.00000 0.00000 0.00016 0.00016 0.00000

 D21 -0.00016 0.00001 0.00000 0.00016 0.00016 0.00000

 D22 3.14140 0.00001 0.00000 0.00019 0.00019 3.14159

 D23 -3.14150 0.00000 0.00000 -0.00009 -0.00009 3.14159

 D24 0.00006 0.00000 0.00000 -0.00006 -0.00006 0.00000

 D25 -0.00011 0.00000 0.00000 0.00011 0.00011 0.00000

 D26 -3.14152 0.00000 0.00000 -0.00007 -0.00007 3.14159

 D27 3.14151 0.00000 0.00000 0.00008 0.00008 3.14159

 D28 0.00010 0.00000 0.00000 -0.00010 -0.00010 0.00000

 D29 0.00034 -0.00001 0.00000 -0.00034 -0.00034 0.00000

 D30 -3.14157 0.00000 0.00000 -0.00002 -0.00002 3.14159

 D31 -3.14144 -0.00001 0.00000 -0.00015 -0.00015 -3.14159

 D32 -0.00016 0.00001 0.00000 0.00016 0.00016 0.00000

 D33 0.00011 -0.00001 0.00000 -0.00011 -0.00011 0.00000

 D34 3.14157 0.00000 0.00000 0.00003 0.00003 3.14159

 D35 -0.00008 0.00000 0.00000 0.00008 0.00008 0.00000

 D36 -3.14147 0.00000 0.00000 -0.00012 -0.00012 3.14159

 D37 -1.06039 0.00000 0.00000 -0.00017 -0.00017 -1.06056

 D38 -3.14148 0.00000 0.00000 -0.00011 -0.00011 3.14159

 D39 1.06071 0.00000 0.00000 -0.00015 -0.00015 1.06056

 D40 2.08096 0.00000 0.00000 0.00007 0.00007 2.08103

 D41 -0.00013 0.00000 0.00000 0.00013 0.00013 0.00000

 D42 -2.08112 0.00000 0.00000 0.00009 0.00009 -2.08103

 Item Value Threshold Converged?

 Maximum Force 0.000047 0.000450 YES

 RMS Force 0.000011 0.000300 YES

 Maximum Displacement 0.000644 0.001800 YES

 RMS Displacement 0.000179 0.001200 YES

 Predicted change in Energy=-3.257444D-08

 Optimization completed.

 -- Stationary point found.

**c) 1-naphthyl isocyanate**

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 - Thermochemistry -

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 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 6 and mass 12.00000

 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 6 and mass 12.00000

 Atom 10 has atomic number 6 and mass 12.00000

 Atom 11 has atomic number 6 and mass 12.00000

 Atom 12 has atomic number 7 and mass 14.00307

 Atom 13 has atomic number 8 and mass 15.99491

 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

 Molecular mass: 169.05276 amu.

 Principal axes and moments of inertia in atomic units:

 1 2 3

 EIGENVALUES -- 1234.229333050.919114285.14844

 X -0.50195 0.86490 0.00000

 Y 0.86490 0.50195 0.00000

 Z 0.00000 0.00000 1.00000

 This molecule is an asymmetric top.

 Rotational symmetry number 1.

 Warning -- assumption of classical behavior for rotation

 may cause significant error

 Rotational temperatures (Kelvin) 0.07018 0.02839 0.02021

 Rotational constants (GHZ): 1.46224 0.59154 0.42116

 Zero-point vibrational energy 399331.8 (Joules/Mol)

 95.44260 (Kcal/Mol)

 Warning -- explicit consideration of 15 degrees of freedom as

 vibrations may cause significant error

 Vibrational temperatures: 93.75 105.33 229.51 261.74 384.55

 (Kelvin) 406.08 625.00 629.77 684.50 704.27

 770.91 791.22 805.94 857.96 886.35

 976.95 1027.59 1094.49 1167.05 1187.94

 1212.90 1253.73 1311.44 1359.21 1436.61

 1469.33 1486.05 1489.76 1507.16 1587.45

 1716.19 1739.73 1754.61 1801.20 1819.28

 1887.99 1969.59 1989.63 2065.63 2145.67

 2164.05 2200.70 2229.01 2301.46 2345.26

 2378.93 3429.25 4588.11 4596.60 4605.60

 4615.57 4625.96 4636.05 4646.44

 Zero-point correction= 0.152097 (Hartree/Particle)

 Thermal correction to Energy= 0.161571

 Thermal correction to Enthalpy= 0.162515

 Thermal correction to Gibbs Free Energy= 0.116405

 Sum of electronic and zero-point Energies= -550.171205

 Sum of electronic and thermal Energies= -550.161731

 Sum of electronic and thermal Enthalpies= -550.160787

 Sum of electronic and thermal Free Energies= -550.206898

 E (Thermal) CV S

 KCal/Mol Cal/Mol-Kelvin Cal/Mol-Kelvin

 Total 101.387 37.458 97.047

 Electronic 0.000 0.000 0.000

 Translational 0.889 2.981 41.283

 Rotational 0.889 2.981 31.157

 Vibrational 99.610 31.496 24.607

 Vibration 1 0.597 1.971 4.294

 Vibration 2 0.599 1.967 4.065

 Vibration 3 0.621 1.892 2.556

 Vibration 4 0.630 1.864 2.309

 Vibration 5 0.672 1.733 1.614

 Vibration 6 0.681 1.707 1.520

 Vibration 7 0.795 1.395 0.844

 Vibration 8 0.798 1.388 0.834

 Vibration 9 0.832 1.304 0.722

 Vibration 10 0.845 1.273 0.685

 Vibration 11 0.891 1.171 0.574

 Vibration 12 0.905 1.140 0.544

 Vibration 13 0.916 1.118 0.524

 Vibration 14 0.954 1.040 0.456

 Vibration 15 0.976 0.998 0.423

 Q Log10(Q) Ln(Q)

 Total Bot 0.286783D-53 -53.542447 -123.286040

 Total V=0 0.261448D+17 16.417385 37.802426

 Vib (Bot) 0.230846D-67 -67.636678 -155.739206

 Vib (Bot) 1 0.316711D+01 0.500663 1.152820

 Vib (Bot) 2 0.281604D+01 0.449638 1.035331

 Vib (Bot) 3 0.126757D+01 0.102972 0.237101

 Vib (Bot) 4 0.110332D+01 0.042703 0.098327

 Vib (Bot) 5 0.724083D+00 -0.140211 -0.322849

 Vib (Bot) 6 0.680401D+00 -0.167235 -0.385073

 Vib (Bot) 7 0.399725D+00 -0.398239 -0.916979

 Vib (Bot) 8 0.395660D+00 -0.402678 -0.927201

 Vib (Bot) 9 0.352823D+00 -0.452443 -1.041789

 Vib (Bot) 10 0.338882D+00 -0.469952 -1.082104

 Vib (Bot) 11 0.296862D+00 -0.527445 -1.214487

 Vib (Bot) 12 0.285392D+00 -0.544558 -1.253891

 Vib (Bot) 13 0.277422D+00 -0.556859 -1.282216

 Vib (Bot) 14 0.251352D+00 -0.599717 -1.380900

 Vib (Bot) 15 0.238378D+00 -0.622734 -1.433898

 Vib (V=0) 0.210452D+03 2.323154 5.349259

 Vib (V=0) 1 0.370634D+01 0.568945 1.310044

 Vib (V=0) 2 0.336008D+01 0.526350 1.211965

 Vib (V=0) 3 0.186262D+01 0.270124 0.621984

 Vib (V=0) 4 0.171133D+01 0.233334 0.537271

 Vib (V=0) 5 0.137994D+01 0.139861 0.322041

 Vib (V=0) 6 0.134436D+01 0.128516 0.295919

 Vib (V=0) 7 0.114014D+01 0.056958 0.131152

 Vib (V=0) 8 0.113761D+01 0.055993 0.128930

 Vib (V=0) 9 0.111195D+01 0.046086 0.106116

 Vib (V=0) 10 0.110402D+01 0.042977 0.098959

 Vib (V=0) 11 0.108149D+01 0.034021 0.078337

 Vib (V=0) 12 0.107572D+01 0.031698 0.072986

 Vib (V=0) 13 0.107181D+01 0.030116 0.069346

 Vib (V=0) 14 0.105962D+01 0.025151 0.057913

 Vib (V=0) 15 0.105392D+01 0.022806 0.052514

 Electronic 0.100000D+01 0.000000 0.000000

 Translational 0.863950D+08 7.936489 18.274440

 Rotational 0.143795D+07 6.157743 14.178726

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

 -------------------------------------------------------------------

 Center Atomic Forces (Hartrees/Bohr)

 Number Number X Y Z

 -------------------------------------------------------------------

 1 6 0.000002375 0.000002561 0.000000000

 2 6 0.000004637 0.000004063 0.000000000

 3 6 -0.000000528 0.000006133 0.000000000

 4 6 0.000000896 0.000003942 0.000000000

 5 6 -0.000004578 0.000007002 0.000000000

 6 6 0.000003273 -0.000000991 0.000000000

 7 6 -0.000010791 0.000010251 0.000000000

 8 6 -0.000001108 -0.000022727 0.000000000

 9 6 -0.000020487 -0.000001129 0.000000000

 10 6 0.000014235 -0.000004041 0.000000000

 11 6 -0.000002986 0.000000447 0.000000000

 12 7 0.000020383 -0.000001738 0.000000000

 13 8 0.000000379 -0.000011635 0.000000000

 14 1 0.000006227 -0.000001448 0.000000000

 15 1 0.000004702 0.000004584 0.000000000

 16 1 0.000001350 0.000008408 0.000000000

 17 1 -0.000002688 0.000005291 0.000000000

 18 1 -0.000003853 0.000000663 0.000000000

 19 1 -0.000009130 -0.000003559 0.000000000

 20 1 -0.000002309 -0.000006077 0.000000000

 -------------------------------------------------------------------

 Cartesian Forces: Max 0.000022727 RMS 0.000006421

 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

 Berny optimization.

 Internal Forces: Max 0.000022412 RMS 0.000003816

 Search for a local minimum.

 Step number 1 out of a maximum of 2

 All quantities printed in internal units (Hartrees-Bohrs-Radians)

 Second derivative matrix not updated -- analytic derivatives used.

 Eigenvalues --- 0.00357 0.00567 0.01468 0.01540 0.01747

 Eigenvalues --- 0.01791 0.02004 0.02169 0.02273 0.02414

 Eigenvalues --- 0.02445 0.02568 0.02579 0.02866 0.02995

 Eigenvalues --- 0.03083 0.03306 0.03566 0.11515 0.11817

 Eigenvalues --- 0.12244 0.12743 0.13114 0.13225 0.13266

 Eigenvalues --- 0.15747 0.18991 0.19799 0.20186 0.20199

 Eigenvalues --- 0.21016 0.21210 0.22311 0.27098 0.28527

 Eigenvalues --- 0.34062 0.36045 0.36219 0.36330 0.36405

 Eigenvalues --- 0.36548 0.36649 0.37058 0.38716 0.39319

 Eigenvalues --- 0.40077 0.43304 0.43834 0.48643 0.48862

 Eigenvalues --- 0.50263 0.51203 0.89069 1.036291000.00000

 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

 Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000

 Angle between quadratic step and forces= 59.01 degrees.

 Linear search not attempted -- first point.

 Iteration 1 RMS(Cart)= 0.00010778 RMS(Int)= 0.00000001

 Iteration 2 RMS(Cart)= 0.00000001 RMS(Int)= 0.00000000

 Variable Old X -DE/DX Delta X Delta X Delta X New X

 (Linear) (Quad) (Total)

 R1 2.60089 0.00000 0.00000 0.00000 0.00000 2.60089

 R2 2.68191 0.00000 0.00000 0.00000 0.00000 2.68191

 R3 2.04544 0.00000 0.00000 0.00000 0.00000 2.04544

 R4 2.67894 0.00000 0.00000 0.00001 0.00001 2.67894

 R5 2.04775 0.00000 0.00000 0.00000 0.00000 2.04775

 R6 2.70873 0.00000 0.00000 0.00001 0.00001 2.70873

 R7 2.70398 0.00000 0.00000 0.00001 0.00001 2.70399

 R8 2.60003 0.00000 0.00000 0.00000 0.00000 2.60003

 R9 2.04789 0.00000 0.00000 0.00000 0.00000 2.04790

 R10 2.68902 0.00001 0.00000 0.00002 0.00002 2.68904

 R11 2.04962 0.00000 0.00000 0.00000 0.00000 2.04962

 R12 2.68622 0.00001 0.00000 0.00001 0.00001 2.68623

 R13 2.61521 0.00002 0.00000 0.00005 0.00005 2.61526

 R14 2.62923 0.00001 0.00000 -0.00001 -0.00001 2.62922

 R15 2.66836 0.00000 0.00000 0.00000 0.00000 2.66837

 R16 2.04658 0.00000 0.00000 0.00000 0.00000 2.04658

 R17 2.60038 -0.00002 0.00000 -0.00004 -0.00004 2.60034

 R18 2.04731 0.00000 0.00000 0.00000 0.00000 2.04731

 R19 2.04876 0.00000 0.00000 0.00000 0.00000 2.04876

 R20 2.27280 -0.00001 0.00000 -0.00004 -0.00004 2.27277

 R21 2.25760 0.00000 0.00000 0.00000 0.00000 2.25761

 A1 2.10542 0.00000 0.00000 0.00000 0.00000 2.10542

 A2 2.11260 0.00000 0.00000 0.00001 0.00001 2.11261

 A3 2.06516 0.00000 0.00000 -0.00001 -0.00001 2.06515

 A4 2.10129 0.00000 0.00000 0.00000 0.00000 2.10129

 A5 2.09578 0.00000 0.00000 0.00001 0.00001 2.09579

 A6 2.08612 0.00000 0.00000 -0.00001 -0.00001 2.08611

 A7 2.08054 0.00000 0.00000 0.00000 0.00000 2.08055

 A8 2.12826 0.00000 0.00000 0.00001 0.00001 2.12827

 A9 2.07438 0.00000 0.00000 -0.00001 -0.00001 2.07436

 A10 2.09911 0.00000 0.00000 0.00000 0.00000 2.09911

 A11 2.08663 0.00000 0.00000 -0.00001 -0.00001 2.08662

 A12 2.09744 0.00000 0.00000 0.00001 0.00001 2.09745

 A13 2.10967 0.00000 0.00000 0.00000 0.00000 2.10968

 A14 2.10556 0.00000 0.00000 0.00000 0.00000 2.10556

 A15 2.06795 0.00000 0.00000 0.00000 0.00000 2.06795

 A16 2.07033 0.00000 0.00000 -0.00001 -0.00001 2.07032

 A17 2.08264 0.00000 0.00000 0.00001 0.00001 2.08265

 A18 2.13021 0.00000 0.00000 0.00000 0.00000 2.13021

 A19 2.09531 0.00000 0.00000 -0.00001 -0.00001 2.09530

 A20 2.06038 0.00000 0.00000 0.00001 0.00001 2.06039

 A21 2.12750 0.00000 0.00000 0.00000 0.00000 2.12750

 A22 2.10612 0.00000 0.00000 0.00000 0.00000 2.10612

 A23 2.08676 0.00000 0.00000 -0.00001 -0.00001 2.08675

 A24 2.09030 0.00000 0.00000 0.00001 0.00001 2.09031

 A25 2.10628 0.00000 0.00000 0.00000 0.00000 2.10627

 A26 2.07623 0.00000 0.00000 0.00002 0.00002 2.07624

 A27 2.10068 0.00000 0.00000 -0.00002 -0.00002 2.10067

 A28 2.10164 0.00000 0.00000 0.00001 0.00001 2.10166

 A29 2.07510 0.00000 0.00000 0.00001 0.00001 2.07510

 A30 2.10644 0.00000 0.00000 -0.00002 -0.00002 2.10642

 A31 2.56651 0.00001 0.00000 0.00030 0.00030 2.56680

 A32 3.24931 0.00000 0.00000 -0.00006 -0.00006 3.24925

 A33 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D1 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D2 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D3 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D4 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D5 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D6 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D7 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D8 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D9 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D10 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D11 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D12 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D13 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D14 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D15 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D16 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D17 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D18 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D19 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D20 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D21 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D22 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D23 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D24 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D25 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D26 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D27 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D28 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D29 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D30 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D31 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D32 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D33 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D34 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D35 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D36 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D37 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D38 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D39 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D40 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D41 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D42 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D43 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D44 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D45 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D46 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 Item Value Threshold Converged?

 Maximum Force 0.000022 0.000450 YES

 RMS Force 0.000004 0.000300 YES

 Maximum Displacement 0.000778 0.001800 YES

 RMS Displacement 0.000108 0.001200 YES

 Predicted change in Energy=-3.110932D-09

 Optimization completed.

 -- Stationary point found.