

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.217569 | 0.183926  | 1.231232  |
| C | 1.217569  | -0.183926 | -1.231232 |
| C | 1.101498  | 1.176729  | 0.895944  |
| H | -0.613648 | -0.402375 | 1.927151  |
| H | 0.613648  | 0.402375  | -1.927151 |
| H | -2.019705 | 0.682185  | 1.778262  |
| H | 2.019705  | -0.682185 | -1.778262 |
| H | 1.426626  | 2.191635  | 1.127390  |
| H | 1.291077  | 0.533323  | 1.760324  |
| C | -1.101498 | -1.176729 | -0.895944 |
| H | -1.291077 | -0.533323 | -1.760324 |
| H | -1.426626 | -2.191634 | -1.127390 |
| N | 1.850834  | 0.703704  | -0.278026 |
| N | -1.850834 | -0.703703 | 0.278026  |
| N | 0.309520  | -1.145254 | -0.628779 |
| N | -0.309520 | 1.145254  | 0.628779  |
| N | -0.856750 | 2.168193  | -0.126498 |
| N | -3.207457 | -0.480385 | 0.016423  |
| N | 0.856750  | -2.168193 | 0.126498  |
| N | 3.207457  | 0.480385  | -0.016423 |
| O | -3.600134 | -0.870725 | -1.079579 |
| O | 3.880229  | -0.011359 | -0.907938 |
| O | 3.600135  | 0.870724  | 1.079579  |
| O | -3.880230 | 0.011359  | 0.907937  |
| O | -2.072586 | 2.118333  | -0.291892 |
| O | -0.075576 | 2.995085  | -0.583426 |
| O | 2.072586  | -2.118332 | 0.291892  |
| O | 0.075576  | -2.995085 | 0.583426  |

Vibrational frequencies (cm<sup>-1</sup>):

|        |        |        |        |        |        |        |
|--------|--------|--------|--------|--------|--------|--------|
| 26.4   | 61.1   | 70.5   | 72.6   | 81.4   | 98.8   | 106.1  |
| 117.5  | 130.6  | 164.5  | 192.9  | 230.8  | 247.3  | 273.2  |
| 311.1  | 332.8  | 361.1  | 368.3  | 413.4  | 416.9  | 425.0  |
| 427.5  | 598.3  | 600.2  | 636.8  | 654.8  | 671.5  | 676.8  |
| 738.4  | 746.2  | 746.9  | 749.4  | 754.7  | 797.7  | 868.9  |
| 873.7  | 895.2  | 905.6  | 961.2  | 970.4  | 992.4  | 993.5  |
| 1101.6 | 1121.0 | 1190.8 | 1212.3 | 1267.5 | 1272.6 | 1287.7 |
| 1293.7 | 1315.4 | 1330.3 | 1344.7 | 1369.2 | 1377.2 | 1379.1 |
| 1393.4 | 1399.7 | 1411.5 | 1442.1 | 1449.8 | 1466.8 | 1490.6 |
| 1492.4 | 1512.8 | 1513.5 | 1772.7 | 1776.7 | 1791.8 | 1792.2 |
| 3108.3 | 3108.9 | 3126.8 | 3126.9 | 3182.7 | 3182.9 | 3190.9 |
| 3191.1 |        |        |        |        |        |        |

Vibrational temperatures (K):

|       |       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|-------|
| 37.9  | 87.9  | 101.4 | 104.5 | 117.1 | 142.2 | 152.6 |
| 169.1 | 187.9 | 236.7 | 277.5 | 332.1 | 355.8 | 393.1 |
| 447.6 | 478.8 | 519.6 | 529.9 | 594.8 | 599.8 | 611.4 |

|        |        |        |        |        |        |        |
|--------|--------|--------|--------|--------|--------|--------|
| 615.1  | 860.9  | 863.6  | 916.2  | 942.1  | 966.2  | 973.8  |
| 1062.5 | 1073.6 | 1074.6 | 1078.2 | 1085.8 | 1147.7 | 1250.1 |
| 1257.0 | 1287.9 | 1302.9 | 1383.0 | 1396.2 | 1427.8 | 1429.5 |
| 1585.0 | 1612.8 | 1713.3 | 1744.2 | 1823.7 | 1831.0 | 1852.7 |
| 1861.3 | 1892.6 | 1914.1 | 1934.7 | 1969.9 | 1981.6 | 1984.3 |
| 2004.8 | 2013.8 | 2030.8 | 2074.9 | 2085.9 | 2110.5 | 2144.7 |
| 2147.2 | 2176.5 | 2177.6 | 2550.6 | 2556.3 | 2578.0 | 2578.5 |
| 4472.1 | 4473.0 | 4498.8 | 4499.0 | 4579.3 | 4579.4 | 4591.0 |
| 4591.3 |        |        |        |        |        |        |

Rotational constants (cm-1): 0.00762 0.00997 0.01964  
 (GHz): 0.22853 0.29875 0.58877

Moments of inertia (a.u.) : \*\*\*\*\* \*\*\*\*\* \*\*\*\*\*

Rotational temperatures (K): 0.01097 0.01434 0.02826

Zero point energy (kJ/mole) : 511.70120  
 (kcal/mole): 122.29952

|               | E        | Cv       | S        |
|---------------|----------|----------|----------|
|               | kJ/mol   | J/mol-K  | J/mol-K  |
| Electronic    | 0.0000   | 0.0000   | 0.0000   |
| Translational | 3.7184   | 12.4716  | 179.7151 |
| Rotational    | 3.7184   | 12.4716  | 139.5223 |
| Vibrational   | 549.0038 | 233.2124 | 247.5553 |
| TOTAL         | 556.4406 | 258.1556 | 566.7927 |

|               | kcal/mol | cal/mol-K | cal/mol-K |
|---------------|----------|-----------|-----------|
| Electronic    | 0.0000   | 0.0000    | 0.0000    |
| Translational | 0.8887   | 2.9808    | 42.9529   |
| Rotational    | 0.8887   | 2.9808    | 33.3466   |
| Vibrational   | 131.2151 | 55.7391   | 59.1671   |
| TOTAL         | 132.9925 | 61.7007   | 135.4667  |

H = 558.9195 kJ/mol

H = 133.5850 kcal/mol

| Temp. | Press. | Enthalpy | Energy   | Heat capacity | Entropy    |
|-------|--------|----------|----------|---------------|------------|
| K     | Atm    | Kcal/mol | Kcal/mol | Kcal/mol-K    | Kcal/mol-K |
| 298.1 | 1.0    | 133.585  | 132.992  | 61.701        | 135.467    |