| | | | |
|---|---|---|---|
| C | -1.273748 | -1.249806 | 1.159577 |
| H | -1.108993 | -1.165579 | 2.240713 |
| H | -2.016321 | -2.017778 | 0.956521 |
| C | 1.273333 | 1.250044 | 1.160111 |
| H | 2.015910 | 2.018043 | 0.957093 |
| H | 1.108049 | 1.166343 | 2.241186 |
| C | 1.272990 | -1.250344 | 1.160099 |
| H | 2.015452 | -2.018406 | 0.956983 |
| H | 1.107878 | -1.166668 | 2.241199 |
| C | -1.273449 | 1.250292 | 1.159388 |
| H | -1.108878 | 1.166322 | 2.240602 |
| H | -2.015713 | 2.018459 | 0.956080 |
| N | 1.775295 | -0.000169 | 0.624399 |
| N | 0.000146 | 1.660710 | 0.602332 |
| N | -0.000320 | -1.660831 | 0.602551 |
| N | -1.775163 | 0.000286 | 0.622731 |
| N | 0.000820 | 1.909874 | -0.778740 |
| N | -0.000131 | -1.910155 | -0.778551 |
| N | -3.123771 | 0.000409 | 0.159569 |
| N | 3.123073 | -0.000214 | 0.159792 |
| O | -3.633642 | 1.092071 | -0.032271 |
| O | -3.633870 | -1.091124 | -0.032420 |
| O | -1.098998 | -2.018544 | -1.304872 |
| O | 1.098960 | -2.017550 | -1.304613 |
| O | 3.632909 | 1.091418 | -0.032516 |
| O | 3.632998 | -1.091773 | -0.032692 |
| O | 1.100238 | 2.017097 | -1.304145 |
| O | -1.097728 | 2.018296 | -1.305764 |

Vibrational frequencies (cm-1):

| | | | | | | |
|---|---|---|---|---|---|---|
| 39.4 | 50.4 | 71.5 | 80.4 | 91.0 | 92.9 | 105.2 |
| 111.7 | 119.2 | 185.9 | 207.2 | 238.3 | 241.3 | 247.3 |
| 336.6 | 397.4 | 397.9 | 406.4 | 413.0 | 425.9 | 464.0 |
| 480.0 | 590.1 | 601.9 | 621.7 | 647.3 | 650.7 | 653.5 |
| 714.9 | 739.2 | 741.4 | 759.6 | 761.4 | 770.6 | 869.1 |
| 869.4 | 889.8 | 891.2 | 910.2 | 932.9 | 954.3 | 960.6 |
| 1054.6 | 1100.2 | 1138.2 | 1217.2 | 1257.9 | 1276.5 | 1300.7 |
| 1301.0 | 1305.3 | 1310.1 | 1332.8 | 1364.0 | 1381.2 | 1384.9 |
| 1406.8 | 1417.2 | 1421.5 | 1428.4 | 1447.6 | 1460.7 | 1473.1 |
| 1481.8 | 1493.9 | 1501.2 | 1795.8 | 1805.3 | 1809.7 | 1811.9 |
| 3079.9 | 3081.6 | 3092.8 | 3093.9 | 3212.7 | 3213.5 | 3214.0 |
| 3214.7 | | | | | | |

Vibrational temperatures (K):

| | | | | | | |
|---|---|---|---|---|---|---|
| 56.6 | 72.5 | 102.9 | 115.7 | 130.9 | 133.7 | 151.3 |
| 160.8 | 171.4 | 267.5 | 298.1 | 342.9 | 347.2 | 355.7 |
| 484.3 | 571.8 | 572.4 | 584.8 | 594.2 | 612.7 | 667.5 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 690.6 | 849.1 | 866.0 | 894.5 | 931.4 | 936.3 | 940.2 |
| 1028.5 | 1063.6 | 1066.8 | 1092.9 | 1095.6 | 1108.8 | 1250.4 |
| 1250.9 | 1280.2 | 1282.2 | 1309.6 | 1342.3 | 1373.0 | 1382.1 |
| 1517.4 | 1583.0 | 1637.6 | 1751.3 | 1809.9 | 1836.7 | 1871.4 |
| 1871.9 | 1878.0 | 1884.9 | 1917.6 | 1962.5 | 1987.3 | 1992.5 |
| 2024.0 | 2039.0 | 2045.2 | 2055.2 | 2082.8 | 2101.6 | 2119.5 |
| 2132.0 | 2149.4 | 2159.9 | 2583.7 | 2597.5 | 2603.8 | 2607.0 |
| 4431.3 | 4433.7 | 4449.9 | 4451.4 | 4622.4 | 4623.6 | 4624.3 |
| 4625.3 | | | | | | |

Rotational constants (cm-1): 0.00845 0.01041 0.01985
(GHz) : 0.25324 0.31219 0.59501
Moments of inertia (a.u.) : ********* ********* *********
Rotational temperatures (K): 0.01215 0.01498 0.02856
Zero point energy (kJ/mole) : 510.89691
(kcal/mole): 122.10729

| | 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 | 138.8688 |
| Vibrational | 547.7023 | 233.2256 | 241.7419 |
| TOTAL | 555.1391 | 258.1688 | 560.3259 |

| | 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 | 33.1904 |
| Vibrational | 130.9040 | 55.7423 | 57.7777 |
| TOTAL | 132.6814 | 61.7038 | 133.9211 |

H = 557.6180 kJ/mol
H = 133.2739 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 | 133.274 | 132.681 | 61.704 | 133.921 |