

C	0.527291	-0.983937	1.302837
C	-0.762567	-0.494648	-0.754861
C	-1.467723	1.593494	0.643562
H	1.115451	-1.809173	1.704297
H	-0.193287	-0.655723	2.057157
H	-1.648448	1.474387	1.715524
H	0.007104	0.155631	-1.178091
H	-1.263627	-1.016967	-1.565659
H	-2.152505	2.345401	0.252329
C	0.949571	1.520939	1.335490
H	1.818865	2.169566	1.251718
H	0.559566	1.552950	2.355703
N	-1.717871	0.314612	-0.047292
N	-0.206346	-1.490812	0.155513
N	1.367536	0.169668	1.044574
N	-0.114625	2.039830	0.491279
N	-2.944782	-0.261908	0.224511
N	2.561861	-0.047158	0.346212
N	0.244668	2.499380	-0.791084
N	0.368947	-2.621884	-0.473538
O	-3.693213	0.400408	0.944233
O	-3.177797	-1.355556	-0.273962
O	-0.678159	2.705929	-1.567461
O	1.438895	2.666630	-0.990490
O	0.863934	-3.453686	0.267705
O	0.259170	-2.684269	-1.690790
O	3.358263	0.875282	0.287866
O	2.690601	-1.174460	-0.120242

Vibrational frequencies (cm⁻¹):

9.8	50.3	51.5	63.0	85.7	100.6	116.7
123.6	134.4	160.1	173.3	189.6	223.9	286.7
304.6	354.3	389.8	402.4	437.7	450.0	460.1
480.0	596.2	617.7	621.8	632.0	655.3	691.7
724.8	737.3	741.2	747.6	761.3	763.8	869.8
880.4	885.0	891.7	946.4	950.2	957.9	972.8
1061.6	1106.0	1178.2	1213.4	1245.4	1277.7	1292.4
1306.4	1313.6	1324.5	1340.3	1367.5	1373.4	1375.6
1395.8	1400.1	1415.7	1429.8	1437.6	1460.5	1477.3
1489.1	1497.0	1511.3	1766.3	1794.8	1803.2	1809.0
3115.3	3118.0	3131.6	3135.3	3189.7	3196.5	3223.1
3224.0						

Vibrational temperatures (K):

14.1	72.4	74.1	90.6	123.3	144.7	168.0
177.8	193.3	230.4	249.3	272.8	322.2	412.5
438.2	509.8	560.9	579.0	629.7	647.5	661.9

690.6	857.8	888.7	894.7	909.2	942.8	995.1
1042.8	1060.8	1066.5	1075.7	1095.4	1098.9	1251.4
1266.7	1273.3	1283.0	1361.7	1367.1	1378.2	1399.7
1527.4	1591.2	1695.1	1745.8	1791.9	1838.4	1859.5
1879.7	1890.0	1905.6	1928.4	1967.5	1976.1	1979.1
2008.3	2014.5	2036.9	2057.1	2068.4	2101.3	2125.5
2142.4	2153.9	2174.4	2541.4	2582.3	2594.4	2602.7
4482.2	4486.2	4505.8	4511.0	4589.3	4599.1	4637.3
4638.7						

Rotational constants (cm-1): 0.00824 0.01295 0.01406
 (GHz): 0.24697 0.38823 0.42163

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

Rotational temperatures (K): 0.01185 0.01863 0.02024

Zero point energy (kJ/mole) : 511.33997
 (kcal/mole): 122.21318

	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	139.4987
Vibrational	548.7382	233.1132	259.5892
TOTAL	556.1750	258.0564	578.8030

	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	33.3410
Vibrational	131.1516	55.7154	62.0433
TOTAL	132.9290	61.6770	138.3372

H = 558.6540 kJ/mol

H = 133.5215 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	133.522	132.929	61.677	138.337