

/1_3_5_7_tetraax_twist_BB

C	0.343440	-1.542220	-0.788687
C	-0.344921	0.788749	-1.542846
H	1.265807	-1.917391	-0.345718
H	-1.268148	0.346416	-1.916585
H	0.015344	1.530976	-2.253302
H	-0.017296	-2.251881	-1.531461
C	-0.345424	-0.787521	1.541605
H	0.014757	-1.530732	2.251105
H	-1.267331	-0.343816	1.916926
C	0.347185	1.542467	0.787032
H	-0.011519	2.252571	1.530359
H	1.269997	1.915948	0.343622
N	-0.642374	1.431637	-0.251349
N	0.643114	-0.250813	-1.430463
N	-0.645347	-1.428384	0.249910
N	0.644528	0.249980	1.427500
N	-1.986758	1.519391	0.126484
N	-1.990047	-1.517895	-0.125332
N	1.988738	-0.126769	1.518291
N	1.987995	0.124643	-1.518478
O	2.812525	-0.769540	-1.375110
O	2.221728	1.302605	-1.771141
O	2.220987	-1.304948	1.771303
O	2.814291	0.766665	1.376130
O	-2.814506	-1.375753	0.769112
O	-2.223824	-1.770242	-1.303355
O	-2.218526	1.771871	1.304866
O	-2.812855	1.376536	-0.766304

Vibrational frequencies (cm-1):

64.3	72.8	73.1	84.6	97.0	99.4	122.1
122.1	147.2	157.7	204.1	227.1	227.2	279.9
299.6	337.4	337.6	386.4	436.8	439.8	439.9
445.4	600.2	619.1	619.2	622.2	650.5	709.0
709.0	746.8	751.8	751.8	754.7	790.3	870.9
871.0	880.4	882.6	935.5	943.8	943.8	962.1
1072.3	1136.8	1136.9	1244.3	1261.6	1272.2	1275.6
1275.8	1323.1	1323.2	1327.1	1343.4	1357.4	1384.5
1384.5	1401.3	1429.3	1430.7	1430.7	1453.3	1509.3
1513.3	1513.4	1516.6	1773.4	1776.6	1782.1	1782.1
3153.0	3153.3	3153.4	3154.2	3214.6	3215.2	3215.3
3216.5						

Vibrational temperatures (K):

92.4	104.8	105.1	121.7	139.6	143.1	175.6
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175.6	211.7	226.8	293.6	326.7	326.9	402.7
431.1	485.4	485.8	556.0	628.4	632.8	632.9
640.8	863.5	890.8	890.9	895.3	935.9	1020.0
1020.1	1074.5	1081.6	1081.7	1085.9	1137.1	1253.1
1253.2	1266.6	1269.9	1346.0	1357.9	1357.9	1384.2
1542.8	1635.6	1635.7	1790.3	1815.1	1830.4	1835.4
1835.5	1903.6	1903.7	1909.4	1932.8	1953.0	1991.9
1992.0	2016.2	2056.5	2058.5	2058.5	2091.0	2171.6
2177.3	2177.4	2182.0	2551.6	2556.1	2564.1	2564.1
4536.4	4537.0	4537.1	4538.3	4625.1	4626.0	4626.2
4627.9						

Rotational constants (cm-1): 0.01100 0.01101 0.01862
 (GHz) : 0.32991 0.32994 0.55810

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

Rotational temperatures (K): 0.01583 0.01583 0.02678

Zero point energy (kJ/mole) : 512.13408
 (kcal/mole): 122.40298

	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	137.8057
Vibrational	548.8869	233.9406	233.6729
TOTAL	556.3237	258.8838	551.1937

	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	32.9364
Vibrational	131.1871	55.9131	55.8492
TOTAL	132.9646	61.8747	131.7385

H = 558.8026 kJ/mol

H = 133.5570 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	133.557	132.965	61.875	131.738