

Harmonic frequencies (cm<sup>-1</sup>), IR intensities (KM/Mole), Raman scattering activities (A<sup>4</sup>/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates:

1					2			3		
B1					B2			A1		
Frequencies	--	1335.3953			1383.4047			1679.2619		
Red. masses	--	1.3687			1.3440			1.1038		
Frc consts	--	1.4380			1.5154			1.8340		
IR Inten	--	0.3735			23.1245			8.6181		
Raman Activ	--	0.7608			4.5167			12.8384		
Depolar (P)	--	0.7500			0.7500			0.5909		
Depolar (U)	--	0.8571			0.8571			0.7429		
Atom AN		X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.17	0.00	0.00	0.00	0.15	0.00	0.00	0.00	0.00
2	8	-0.04	0.00	0.00	0.00	-0.08	0.00	0.00	0.00	0.08
3	1	-0.70	0.00	0.00	0.00	-0.25	-0.65	0.00	-0.35	-0.61
4	1	-0.70	0.00	0.00	0.00	-0.25	0.65	0.00	0.35	-0.61
4					5			6		
A1					A1			B2		
Frequencies	--	2027.5415			3161.4181			3233.7383		
Red. masses	--	7.2562			1.0490			1.1206		
Frc consts	--	17.5752			6.1772			6.9041		
IR Inten	--	150.0223			49.5917			135.4759		
Raman Activ	--	8.1287			137.5987			58.1798		
Depolar (P)	--	0.3281			0.1829			0.7500		
Depolar (U)	--	0.4941			0.3093			0.8571		
Atom AN		X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.00	0.00	0.58	0.00	0.00	0.06	0.00	0.10	0.00
2	8	0.00	0.00	-0.41	0.00	0.00	0.00	0.00	0.00	0.00
3	1	0.00	-0.46	-0.19	0.00	0.61	-0.35	0.00	-0.60	0.37
4	1	0.00	0.46	-0.19	0.00	-0.61	-0.35	0.00	-0.60	-0.37

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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 8 and mass 15.99491

Atom 3 has atomic number 1 and mass 1.00783

Atom 4 has atomic number 1 and mass 1.00783

Molecular mass: 30.01056 amu.

Principal axes and moments of inertia in atomic units:

	1	2	3
EIGENVALUES --	6.15083	44.95434	51.10517
X	0.00000	0.00000	1.00000
Y	0.00000	1.00000	0.00000
Z	1.00000	0.00000	0.00000

This molecule is an asymmetric top.

Rotational symmetry number 2.

Rotational temperatures (Kelvin) 14.08165 1.92671 1.69482

Rotational constants (GHZ): 293.41429 40.14609 35.31426

Zero-point vibrational energy 76685.2 (Joules/Mol)

18.32820 (Kcal/Mol)

Vibrational temperatures: 1921.33 1990.41 2416.08 2917.18 4548.57

(Kelvin) 4652.62

Zero-point correction= 0.029208 (Hartree/Particle)

Thermal correction to Energy= 0.032061

Thermal correction to Enthalpy= 0.033005

Thermal correction to Gibbs Free Energy= 0.008251

Sum of electronic and zero-point Energies= -113.837123

Sum of electronic and thermal Energies= -113.834270

Sum of electronic and thermal Enthalpies= -113.833326

Sum of electronic and thermal Free Energies= -113.858080

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	20.119	6.256	52.100
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	36.130
Rotational	0.889	2.981	15.920
Vibrational	18.341	0.294	0.050
	Q	Log10(Q)	Ln(Q)
Total Bot	0.160331D-03	-3.794983	-8.738271
Total V=0	0.436177D+10	9.639663	22.196144
Vib (Bot)	0.368765D-13	-13.433251	-30.931203
Vib (V=0)	0.100322D+01	0.001395	0.003212
Electronic	0.100000D+01	0.000000	0.000000
Translational	0.646199D+07	6.810366	15.681448
Rotational	0.672824D+03	2.827901	6.511484

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

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