Electronic Supplementary Material (ESI) for RSC Advances.
This journal is © The Royal Society of Chemistry 2016

Electronic Supporting Information

A mechanistic study of carbonyl activation under solvent–free conditions: Evidence drawn from the synthesis of imidazoles

Kiran Pradhan[a], Bipransh Kumar Tiwary[b], Mussaraff Hossain[a], Ranadhir Chakraborty[b], Ashis Kumar Nanda[a]*

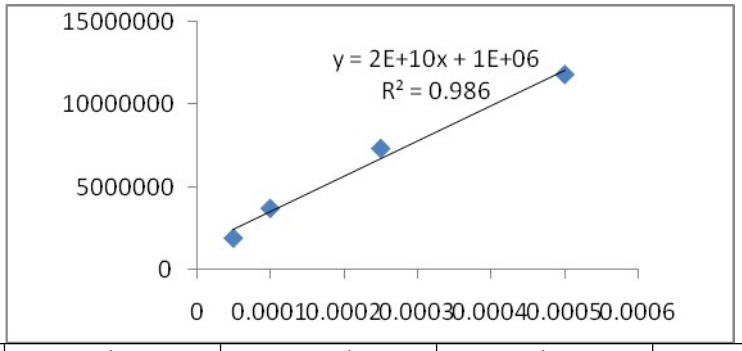
[a]*Department of Chemistry, University of North Bengal, Darjeeling, India, 734013.*
E-mail – ashis_nanda@hotmail.com, Mobile no- +91-9474329191

[b]*Department of Biotechnology, University of North Bengal, Darjeeling, India, 734013*

Kinetic Studies

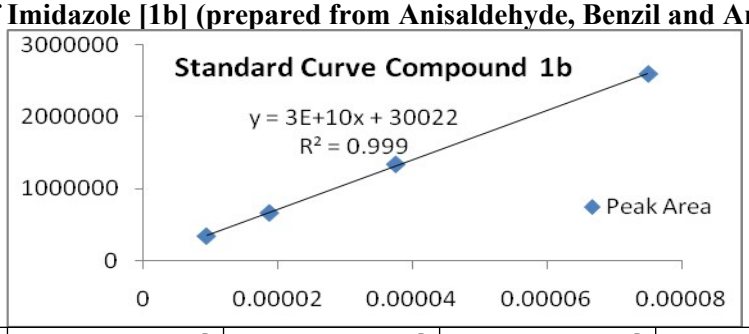
Standard Curve Preparation

Standard curve of Benzil



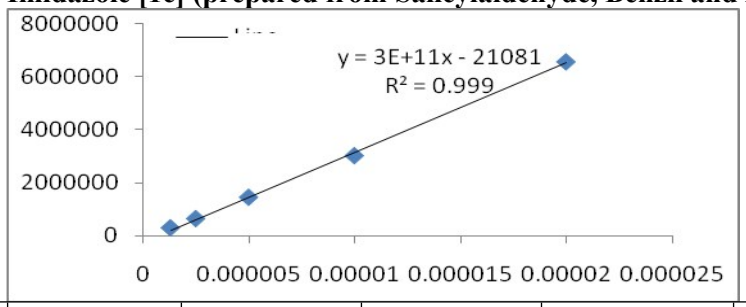
Concentration	5 X 10^{-4}	2.5 X 10^{-4}	1 X 10^{-4}	0.5 X 10^{-4}
Peak Area	11808950	7331784	3704440	1905962

Standard curve of Imidazole [1b] (prepared from Anisaldehyde, Benzil and Ammonium Acetate):



Concentration	7.5 X 10^{-5}	3.75 X 10^{-5}	1.88 X 10^{-5}	9.4 X 10^{-6}
Peak Area	2599295	1342807	668203	345233

Standard curve of Imidazole [1c] (prepared from Salicylaldehyde, Benzil and Ammonium Acetate):



Concentration	2 X 10^{-5}	1 X 10^{-5}	0.5 X 10^{-5}	0.25 X 10^{-5}	0.13 X 10^{-5}
Peak Area	6579714	3027267	1451223	643988	297376

Calculation of Rate constants:

From the slope of the first order rate equation;

$$\frac{dC}{dt} = (+/-)\ kC$$

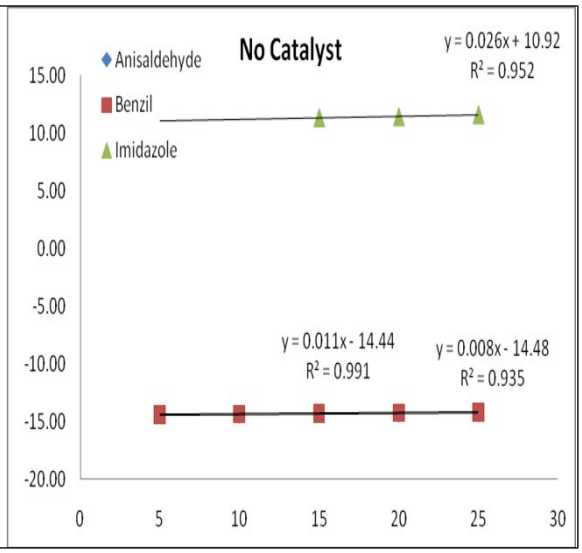
$C \alpha I;\ C = I*X$

$\pm \ln I = (+/-)\ kt + \text{intgn constant}$

the rate constants and $t_{1/2}$ for all the reactions (non-catalysed and catalysed) leading to the formation of the Imidazole was calculated.

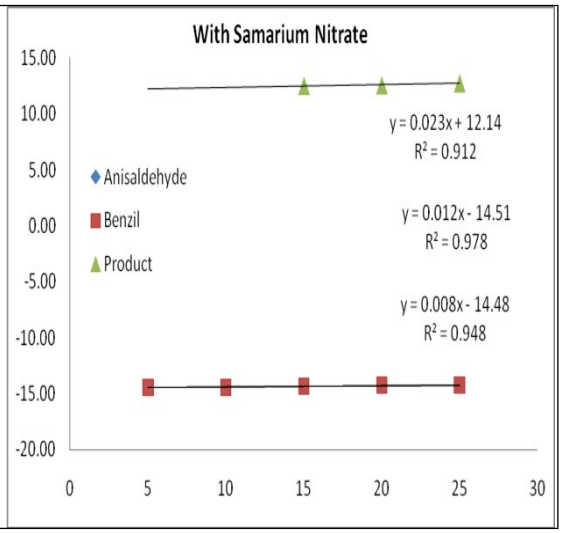
[1] Solvent-free (No Catalyst)

Time (min)	aldehyde	Benzil	Imidazole	-ve ln I	-ve ln I	+ve ln I
5	1887866	1777041	0	-14.45	-14.39	
10	1832777	1678248	0	-14.42	-14.33	
15	1692279	1571646	83968	-14.34	-14.27	11.34
20	1652630	1518525	91098	-14.32	-14.23	11.42
25	1624263	1411489	109493	-14.30	-14.16	11.60



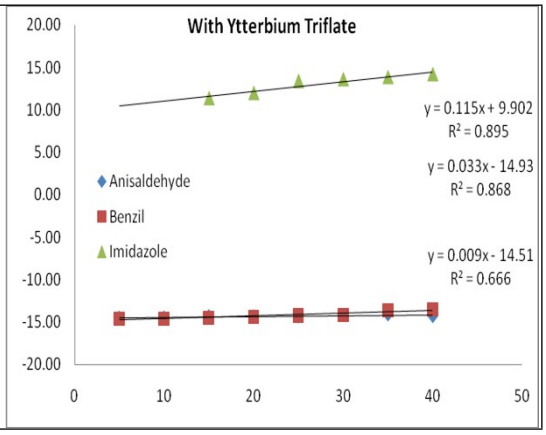
[2] With Samarium Nitrate hexahydrate

Time (min)	aldehyde	Benzil	Imidazole	-ve ln I	-ve ln I	+ve ln I
5	1857401	1868149	0	-14.43	-14.44	
10	1837660	1806170	0	-14.42	-14.41	
15	1723382	1701810	272569	-14.36	-14.35	12.52
20	1622598	1554631	287529	-14.30	-14.26	12.57
25	1598453	1487174	343434	-14.28	-14.21	12.75



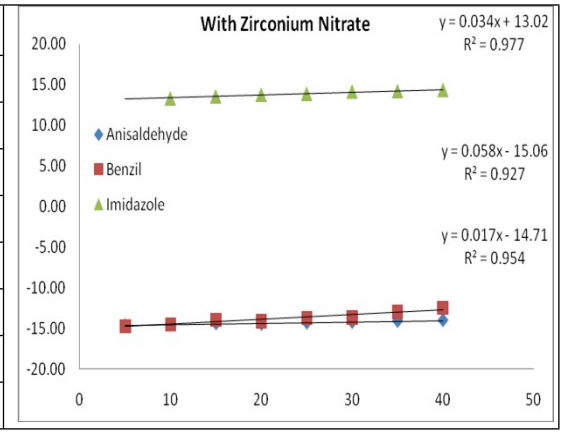
[3] With Ytterbium triflate

Time (min)	aldehyde	Benzil	Imidazole	-ve ln I	-ve ln I	+ve ln I
5	1967276	2176470	0	-14.49	-14.59	
10	1919356	2175832	0	-14.47	-14.59	
15	1642066	1948681	84787	-14.31	-14.48	11.35
20	1676305	1687663	159902	-14.33	-14.34	11.98
25	1672598	1477532	656829	-14.33	-14.21	13.40
30	1405615	1454681	823661	-14.16	-14.19	13.62
35	1588615	763247	1053173	-14.28	-13.55	13.87
40	1305757	713412	1472645	-14.08	-13.48	14.20



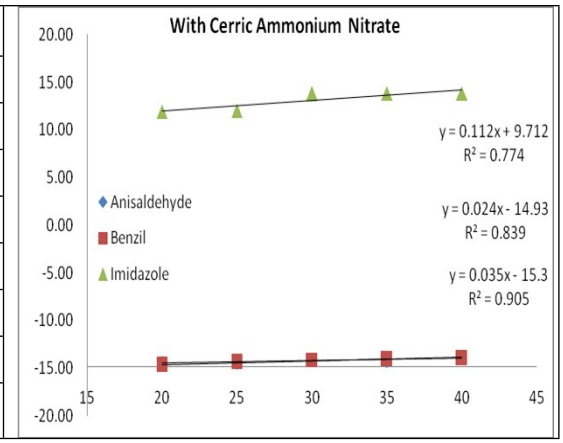
[4] With Zirconium Nitrate

Time min	aldehyde	Benzil	Imidazole	-ve ln I	-ve ln I	+ve ln I
5	2270862	2446728	0	-14.64	-14.71	
10	2067054	1947681	599012	-14.54	-14.48	13.30
15	1735717	1147822	780943	-14.37	-13.95	13.57
20	1889227	1306034	942330	-14.45	-14.08	13.76
25	1605435	890240	1069961	-14.29	-13.70	13.88
30	1471802	842336	1408707	-14.20	-13.64	14.16
35	1311074	433157	1489670	-14.09	-12.98	14.21
40	1196557	261571	1711185	-13.99	-12.47	14.35



[5] With Ceric Ammonium Nitrate

Time (min)	aldehyde	Benzil	Imidazole	-ve ln I	-ve ln I	+ve ln I
5	2326193	2513519	0	-14.66	-14.74	
10	2332837	2373069	0	-14.66		
15	2231400	2353884	0	-14.62		
20	1835503	2388096	149926	-14.42	-14.69	11.92
25	1773508	1737761	166358	-14.39	-14.37	12.02
30	1364423	1335947	967791	-14.13	-14.11	13.78
35	1476913	1281825	995504	-14.21	-14.06	13.81
40	1102140	1144424	1007135	-13.91	-13.95	13.82



[6] With Nickel Chloride Hexahydrate

Time (min)	aldehyde	Benzil	Imidazole	-ve ln I	-ve ln I	+ve ln I
5	2349582	2289395	0	-14.67	-14.64	
10	2181416	2215418	0	-14.60	-14.61	
15	2154692	2091386	0	-14.58	-14.55	
20	1835500	1769201	650785	-14.42	-14.39	13.39
25	1792145	1630789	928681	-14.40	-14.30	13.74
30	1675254	1570751	1078379	-14.33	-14.27	13.89
35	1498372	1401578	1309883	-14.22	-14.15	14.09
40	952029	526652	1552614	-13.77	-13.17	14.26

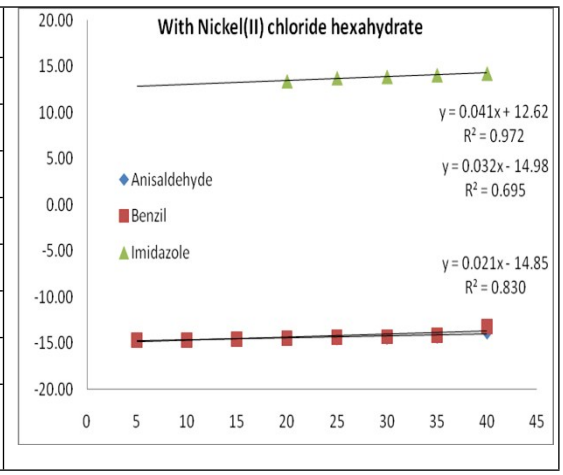


Figure S1 Temperature Optimisation for maximum conversion: HPLC Peak Area vs Temp. after 20 mins of reaction (Compound **[1b]** via Scheme 1)

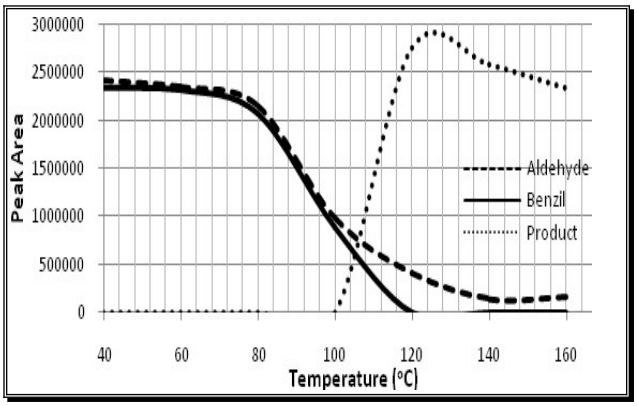


Figure S2 Comparison of percentage yield of Imidazole, **[1b]** at 140°C, 160°C and benzil consumption at 140°C versus time (mins)

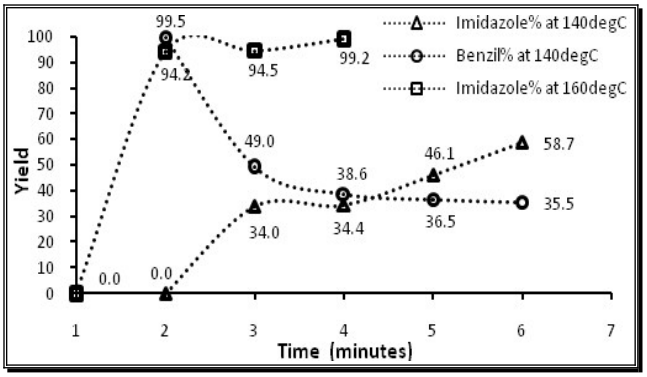
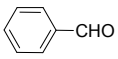
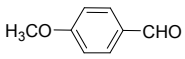
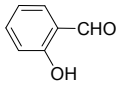
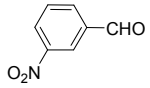
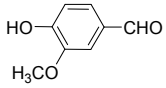
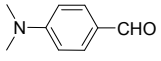
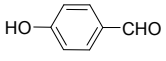
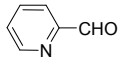
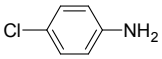
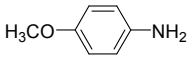
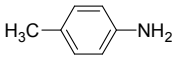
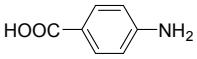
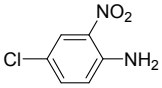
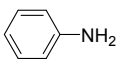
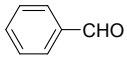
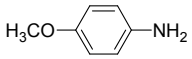
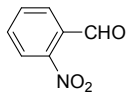
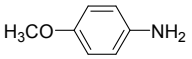
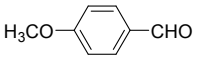
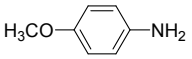
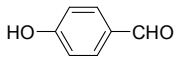


Table S1 Solvent free synthesis of 2,4,5-trisubstituted Imidazoles

Entry	Aldehyde (R-CHO)	Product	Melting Point / °C	Yield%[a]
1		**[1a]**	274-276	99
2		**[1b]**	226-228	98
3		**[1c]**	202-203	98
4		**[1d]**	> 300	99
5		**[1e]**	165-168	97
6		**[1f]**	256-258	97
7		**[1g]**	260-261	98
8		**[1h]**	240-242	99
9		**[1i]**	225-226	99

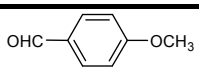
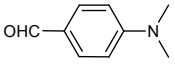
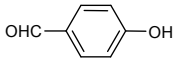
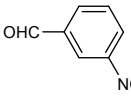
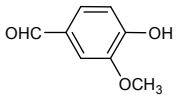
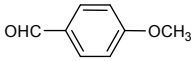
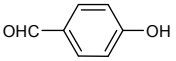
[a] Determined from HPLC peak area count with respect to the purified product

Table S2 Solvent free synthesis of 1,2,4,5-tetrasubstituted Imidazoles

Entry	Amine (R_1-NH_2)	Aldehyde (R_2-CHO)	Product	Melting Point / °C	Yield %[a]
1	$CH_3CH_2CH_2CH_2NH_2$		**[2a]**	78-80	98
2			**[2b]**	209-211	99
3			**[2c]**	180-182	99
4			**[2d]**	218-220	99
5			**[2e]**	170-172	98
6			**[2f]**	>270	98
7	NH_2CH_2COOH		**[2g]**	173-175	99
8			**[2h]**	206-208	99
9			**[2i]**	78-80	99
10			**[2j]**	209-211	99
11			**[2k]**	180-182	98
12			**[2l]**	218-220	99

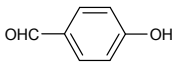
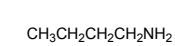
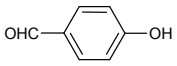
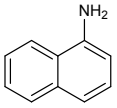
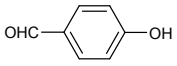
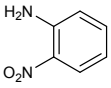
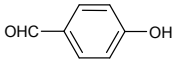
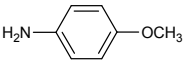
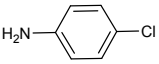
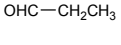
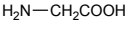
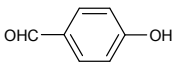
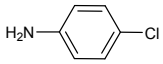
[a] Determined from HPLC peak area count with respect to the purified product

Table S3 Synthesis of Imidazole N-oxides under catalyst-free and solvent-free conditions

Entry	Monoxime	Aldehyde	Product	Melting Point (°C)	Yield %[a]
1	A		**[3a]**	138-140	99
2	A		**[3b]**	233-235	99
3	A		**[3c]]**	>260-270	98
4	A		**[3d]**	172-174	98
5	B		**[3e]**	197-199	99
6	B		**[3f]**	95-96	99
7	B		**[3g]**	230-232	98

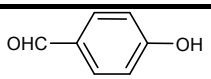
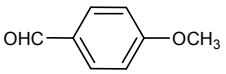
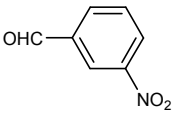
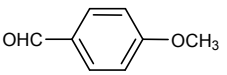
[a] Determined from HPLC peak area count with respect to the purified product

Table S4 Synthesis of N-substituted Imidazole N-oxides under catalyst-free and solvent-free conditions

Entry	Monoxime	Aldehyde	Primary amine	Product	Melting Point	Yield[a]
1	A			**[4a]**	128-130	99
2	A			**[4b]**	232-235	99
3	A			**[4c]**	272-273	98
4	A			**[4d]**	205-207	99
5	B			**[4e]**	238-240	98
6	B			**[4f]**	>260	97
7	B			**[4g]**	182-184	99

[a] Determined from HPLC peak area count with respect to the purified product

Table S5 Synthesis of 1-hydroxyImidazole-3-oxides under catalyst-free and solvent-free conditions

Entry	Monoxime	Aldehyde	Product	Melting Point	Yield %[a]
1	A		**[5a]**	165-168	98
2	A		**[5b]**	196-198	99
3	A		**[5c]**	209-211	99
4	A		**[5f]**	136-137	99
5	B		**[5g]**	233-235	99

[a] Determined from HPLC peak area count with respect to the purified product

Tri-substituted Imidazoles

2, 4, 5-Triphenylimidazole [1a]: M.P. 274-276^{o}C

^{1}HNMR (300 MHz, DMSO): δ 7.30-8.12 (m, $3C_6H_5$); ***^{13}CNMR (75 MHz, DMSO):*** 145.94, 130.83, 129.13, 128.87, 128.68, 128.36, 128.15, 127.73, 125.66; ***IR (KBr, cm^{-1}):*** 3424 (N-H), 3050 (C-H), 1603 (C=C), 1480 (C=N); ***m/z found for ($C_{21}H_{18}N_2$):*** 297.4 (M+1)

Anal. Calc. for ***$C_{21}H_{18}N_2$***: C, 85.11; H, 5.44; N, 9.45. Found: C, 85.32; H, 5.68; N, 9.62

2-(4-methoxyphenyl)-4, 5-diphenylimidazole [1b]: M.P. 226-228^{o}C

^{1}HNMR (300 MHz, DMSO): δ 3.813(s, OCH_3); δ 7.05 (d, 2H); δ 7.03-7.54 (m, 10H, Ph); δ 8.03 (d, 2H): ***^{13}CNMR (75 MHz, DMSO):*** 158.93, 145.07, 127.95, 126.73, 126.22, 122.61, 113.61, 54.72; ***IR (KBr, cm^{-1}):*** 3409(N-H), 3057(C-H), 1616(C=C), 1493(C=N); ***m/z found for ($C_{22}H_{20}N_2O$):*** 329.6(M+1)

Anal. Calc. for ***$C_{22}H_{20}N_2O$***: C, 80.46; H, 6.14; N, 8.53; O, 4.87. Found: C, 80.95; H, 5.68; N, 8.62; O, 4.63

2-(4,5-diphenyl 1H-imidazol-2-yl) phenol [1c]: M.P. 202-203^{o}C

^{1}HNMR (300 MHz, DMSO): δ 7.40-7.66 (m,5H); δ 7.21-7.24 (d,1H); 6.96-6.99 (dd, 1H); δ 6.75-6.77 (dd, 1-H); δ 6.66-6.89 (d, 1H); δ 6.05 (s, 1H); ***^{13}CNMR (75 MHz, DMSO):*** 165.7, 154.2, 134.6, 130.6, 127.8, 127.3, 126.6, 126.0, 117.8, 114.6; ***IR (KBr, cm^{-1}):*** 3278(N-H), 3058 (C-H), 1603 (C=C), 1485(C=N), 1074, 696; ***m/z found for ($C_{21}H_{18}N_2O$):*** 315.5 (M+1).

Anal. Calc. for ***$C_{21}H_{18}N_2O$***: C, 80.23; H, 5.77; N, 8.91; O, 5.09. Found: C, 80.75; H, 5.85; N, 8.85; O, 5.20

2-(3-nitrophenyl)-4,5-diphenylimidazole [1d]: M.P. >300^{o}C

^{1}HNMR (300 MHz, DMSO): δ 13.10 (s, 1H); δ 8.95 (s,1H); δ 8.52 (d, 1H); δ 8.20 (d, 1H); δ 7.77 (d, 1H); δ 7.55-7.39 (m,10H); ***^{13}CNMR (75 MHz, DMSO):*** 147.9, 142.8, 131.4, 130.7, 129.9, 127.9, 127.2, 122.1, 118.9. ***IR (KBr, cm^{-1}):*** 3398(N-H), 3059(C-H), 1603(C=C), 1529(C=N), 1345, 1070, 694; ***m/z found for ($C_{21}H_{17}N_3O_2$):*** 344.2(M+1).

Anal. Calc. for ***$C_{21}H_{17}N_3O_2$***: C, 73.45; H, 4.99; N, 12.24; O, 9.32. Found: C, 73.21; H, 5.09; N, 12.29; O, 9.26

2-(4,5-diphenyl 1H-imidazol-2-yl)-3-methoxy phenol [1e]: M.P. 165-168^{o}C

^{1}HNMR (300 MHz, DMSO): δ 3.86 (s,3H); δ 6.85-6.88 (m, 3H); δ 7.26-7.36 (m, 5-H); δ 7.39-7.64 (m, 5H); δ 12.5 (brs, 1H); ***^{13}CNMR (75 MHz, DMSO):*** 147.2, 146.7, 145.4, 132.6, 127.9, 127.3, 126.6, 121.1, 118.0, 115.1, 108.9, 55.4; ***IR (KBr, cm^{-1}):*** 3503(N-H), 3412 (O-H), 3047 (C-H), 1603 (C=C), 1494(C=N); ***m/z found for ($C_{22}H_{20}N_2O_2$):*** 345.8 (M+1).

Anal. Calc. for ***$C_{22}H_{20}N_2O_2$***: C, 76.72; H, 5.85; N, 8.13; O, 9.29. Found: C, 76.68; H, 5.92; N, 8.31; O, 9.15

{4-(4,5-diphenyl1H-imidazol-2-yl)phenyl}–dimethylamine [1f]: M.P. 256-258^{o}C

[1]HNMR (300 MHz, DMSO): δ 7.89 (d, 1H); δ 7.52 (d,1H); δ 7.28-7.35 (m, 10H); δ 6.80 (d, 1H); δ 3.52 (s, 3H): ***[13]CNMR (75 MHz, DMSO):*** 149.8, 145.9, 127.8, 126.3, 125.8, 117.8, 111.4, 39.8; ***IR (KBr, cm^{-1}):*** 3350(N-H), 3067(C-H), 1614(C=C), 1502(C=N), 1070; ***m/z found for ($C_{23}H_{23}N_3$):*** 342.8(M+1).

Anal. Calc. for ***$C_{23}H_{23}N_3$***: C, 80.90; H, 6.79; N, 12.31. Found: C, 80.95; H, 6.68; N, 12.38

2-(4-hydroxyphenyl)-4, 5-diphenylimidazole [1g]: M.P. 260-261^{o}C

[1]HNMR (300 MHz, DMSO): δ 7.30-7.51 (m, 10H); δ 6.85-6.88 (d, 2H); δ 7.89-7.92(d, 2H); δ 12.58(s, NH); ***[13]CNMR (75 MHz, DMSO):*** 158.23, 146.53, 135.85, 131.79, 129.04, 128.66, 127.55, 127.32, 126.84, 122.07, 115.86; ***IR (KBr, cm^{-1}):*** 3200 (N-H), 3050 (C-H), 1610 (C=C), 1490 (C=N); ***m/z found for ($C_{21}H_{18}N_2O$):*** 315.2(M+1).

Anal. Calcd for ***$C_{21}H_{18}N_2O$***: C, 80.23; H, 5.77; N, 8.91; O, 5.09. Found: C, 80.15; H, 5.78; N, 8.72; O, 4.98

2-(4,5-diphenyl 1H-imidazol-2-yl) pyridine [1h]: M.P. 240-242^{o}C

[1]HNMR (300 MHz, DMSO): δ 8.66 (d,1H); δ 8.14 (d,1H); δ 8.11 (dd, 1H); δ 8.09 (d, 1-H); δ 7.50- 7.29 (m, $2C_6H_5$); ***[13]CNMR (75 MHz, DMSO):*** 149.46, 149.21, 145.92, 137.67, 130.84, 129.14, 128.87, 128.78, 128.37, 127.58, 125.67, 123.63, 120.39; ***IR (KBr, cm^{-1}):*** 3420(N-H), 3058 (C-H), 1602 (C=C), 1489(C=N), 1070, 694; ***m/z found for ($C_{20}H_{17}N_3$):*** 300.8 (M+1).

Anal. Calc. for ***$C_{20}H_{17}N_3$***: C, 80.24; H, 5.72; N, 14.04. Found: C, 80.35; H, 5.59; N, 14.23

4, 5-diphenyl-1-H imidazole [1i]: M.P. 225-226^{o}C

[1]HNMR (300 MHz, $CDCl_3$): δ 7.65 (s,1H); δ 7.50- δ 7.26 (m, $2C_6H_5$); ***[13]CNMR (75 MHz, DMSO):*** 134.54, 132.26, 131.55, 128.66, 127.85, 129.14, 127.64; ***IR (KBr, cm^{-1}):*** 3380 (N-H), 3066 (Ar C-H), 2810 (Al C-H), 1602 (C=C), 1512 (C=N), 1452, 1070, 698; ***m/z found for ($C_{15}H_{12}N_2$):*** 220.10 (M+1).

Anal. Calc. for ***$C_{15}H_{12}N_2$***: C, 81.79; H, 5.49; N, 12.72. Found: C, 81.85; H, 5.52; N, 12.56

Tetra-substituted Imidazoles

1-butyl-4,5-diphenyl-1-H imidazole [2a]. M.P. 78-80^{o}C

[1]HNMR (300 MHz, $CDCl_3$): δ 7.62 (s,1H); δ 7.43-δ 7.20 (m, $2C_6H_5$); δ 3.78 (t,1H); δ 1.56 (m,1H); δ 1.24 (m,1H); δ 0.82 (t,1H); ***[13]CNMR (75 MHz, $CDCl_3$):*** 138.0, 136.62, 134.69, 130.97, 130.85, 129.04, 128.65, 128.50, 128.09, 127.78, 126.55, 126.20; ***IR (KBr, cm^{-1}):*** 3060 (Ar C-H), 2872 (Al C-H), 1601 (C=C), 1506 (C=N), 1448, 1242, 1071, 704; ***m/z found for ($C_{19}H_{20}N_2$):*** 276.2 (M+1).

Anal. Calcd for ***$C_{19}H_{20}N_2$***: C, 82.57; H, 7.29; N, 10.14. Found: C, 81.92; H, 7.45; N, 10.26

1-(4-chlorophenyl)-4,5-diphenyl-1-H imidazole [2b]. M.P. 209-211^{o}C.

[1]HNMR (300 MHz, $CDCl_3$): δ 7.80 (s,1H); δ 7.55-δ 7.03 (m, $3C_6H_5$); ***[13]CNMR (75 MHz, $CDCl_3$):*** 138.86, 137.08, 134.82, 133.99, 133.84, 130.77, 129.61, 129.50, 128.79, 128.58, 128.43, 128.27, 127.25, 126.93.

IR (KBr, cm^{-1}): 3045 (Ar C-H), 1599 (C=C), 1497 (C=N), 1440, 1248, 1091, 698; ***m/z found for ($C_{21}H_{15}ClN_2$):*** 330.2 (M+1).

Anal. Calcd for ***$C_{21}H_{15}ClN_2$***: C, 76.24; H, 4.57; Cl, 10.72; N, 8.47. Found: C, 76.36; H, 4.52; Cl, 10.62; N, 8.52

1-(4-methoxyphenyl)-4, 5-diphenyl-1-H Imidazole [2c]. M.P.180-182^{o}C

^{1}HNMR (300 MHz, $CDCl_3$): δ 7.76 (s,1H); δ 7.76- δ 6.81 (m, $3C_6H_5$); δ 3.79 (s,3H); ***^{13}CNMR (75 MHz, $CDCl_3$):*** 138.33, 137.42, 134.21, 130.81, 130.03, 129.22, 128.96, 128.56, 128.20, 128.10, 127.21, 127.13, 126.69; ***IR (KBr, cm^{-1}):*** 3047 (Ar C-H), 2837 (Al C-H), 1600 (C=C), 1515 (C=N), 1440, 1251, 1070, 698

m/z found for ($C_{22}H_{18}N_2O$): 326.8 (M+1).

Anal. Calc. for ***$C_{22}H_{18}N_2O$***: C, 80.96; H, 5.56; N, 8.58; O, 4.90. Found: C, 80.84; H, 5.45; N, 8.51; O, 4.79

4-(4,5-diphenyl-1H-imidazol-1-yl)phenol [2d]: M.P. 218-220^{o}C.

^{1}HNMR (300 MHz, $CDCl_3$): δ 7.64 (s,1H); δ 7.50-δ 7.26 (m, $3C_6H_5$); δ 4.30 (s,1H); ***^{13}CNMR (75 MHz, $CDCl_3$):*** 134.65, 132.45, 131.62, 128.64, 127.82, 127.55; ***IR (KBr, cm^{-1}):*** 3057 (Ar C-H), 1602 (C=C), 1512 (C=N), 1442, 1248, 1070, 698; ***m/z found for ($C_{21}H_{16}N_2O$):*** 312.1 (M+1).

Anal. Calc. for ***$C_{21}H_{16}N_2O$***: C, 80.75; H, 5.16; N, 8.97; O, 5.12. Found: C, 80.84; H, 5.24; N, 8.78; O, 5.22

4,5-diphenyl-1-p-tolyl-1H-imidazole [2e]: M.P.170-172^{o}C.

^{1}HNMR (300 MHz, $CDCl_3$): δ 7.79 (s,1H); δ 7.56-δ 6.98 (m, $3C_6H_5$); δ 2.34 (s,3H); ***^{13}CNMR (75 MHz, $CDCl_3$):*** 138.44, 138.04, 137.30, 134.13, 133.76, 130.80, 130.01, 129.80, 128.74, 128.57, 128.21, 128.12, 127.24, 126.73, 125.58; ***IR (KBr, cm^{-1}):*** 3105 (Ar C-H), 1600 (C=C), 1515 (C=N), 1440, 1242, 1070, 698.

m/z found for ($C_{22}H_{18}N_2$): 310.3 (M+1).

Anal. Calcd for ***$C_{22}H_{18}N_2$***: C, 85.13; H, 5.85; N, 9.03. Found: C, 85.16; H, 5.82; N, 9.15

4-(4,5-diphenyl-1H-imidazol-1-yl)benzoic acid [2f]:M.P. >270^{o}C.

^{1}HNMR (300 MHz, $CDCl_3$): δ 8.02 (d, 2H); δ 7.48 (s, 1H); δ 7.34-δ 7.18 (m, $2C_6H_5$); δ 3.42 (s,1H); ***^{13}CNMR (75 MHz, $CDCl_3$):*** 167.21, 130.84, 130.68, 128.84, 128.26, 127.19, 125.23; ***IR (KBr, cm^{-1}):*** 3057 (Ar C-H), 2852, 2551, 1683, 1604 (C=C), 1506 (C=N), 1430, 1292, 1070, 696; ***m/z found for ($C_{22}H_{16}N_2O_2$):*** 340.4 (M+1).

Anal. Calc. for ***$C_{22}H_{16}N_2O_2$***: C, 77.63; H, 4.74; N, 8.23; O, 9.40. Found: C, 77.81; H, 4.65; N, 8.19; O, 9.44

2-(4,5-diphenyl-1H-imidazol-1-yl)acetic acid [2g]: M.P. 173-175^{o}C.

^{1}HNMR (300 MHz, $CDCl_3$): δ 7.78 (s,1H); δ 7.56-δ 7.34 (m, $2C_6H_5$); δ 4.30 (s,1H); δ 3.50 (s,2H); ***^{13}CNMR (75 MHz, $CDCl_3$):*** 148.77, 138.46, 131.08, 130.06, 129.33, 129.23, 128.90, 128.76, 128.46, 127.92, 127.41, 126.35; ***IR (KBr, cm^{-1}):*** 3055 (Ar C-H), 2825 (Al C-H), 1686, 1602 (C=C), 1506 (C=N), 1393, 1211, 1072, 696.

m/z found for ($C_{17}H_{14}N_2O_2$): 278.5 (M+1).

Anal. Calcd for ***$C_{17}H_{14}N_2O_2$***: C, 73.37; H, 5.07; N, 10.07; O, 11.50. Found: C, 73.54; H, 4.95; N, 10.19; O, 11.52

1-(4-chloro-2-nitrophenyl)-4,5-diphenyl-1H-imidazole [2h]: M.P. 206-208^{o}C.

^{1}HNMR (300 MHz, $CDCl_3$): δ 7.80 (s,1H); δ 7.46-δ 7.28 (m, 14H); ***^{13}CNMR (75 MHz, $CDCl_3$):*** 142.86, 137.08, 135.82, 133.99, 133.84, 130.77, 129.61, 129.32, 128.79, 128.58, 127.43, 123.27; ***IR (KBr, cm^{-1}):*** 3060(Ar C-H), 1652, 1602 (C=C), 1510 (C=N), 1442, 1070; ***m/z found for ($C_{21}H_{14}ClN_3O_2$):*** 375.8 (M+1).

Anal. Calc. for ***$C_{21}H_{14}ClN_3O_2$***: C, 67.12; H, 3.75; Cl, 9.43; N, 11.18; O, 8.51. Found: C, 67.10; H, 3.69; Cl, 9.62; N, 11.20; O, 8.59

1,2,4,5-tetraphenyl-1H-imidazole [2i]: M.P. 215-217^{o}C

^{1}HNMR (300 MHz, $CDCl_3$): δ 7.61-δ 7.07 (m, 12H); ***^{13}CNMR (75 MHz, $CDCl_3$):*** 146.91, 138.20, 137.04, 134.33, 131.10, 130.83, 130.57, 130.41, 129.02, 128.96, 128.40, 128.33, 12.28, 128.15, 128.09, 127.96, 127.41, 126.62; ***IR (KBr, cm^{-1}):*** 3057(Ar C-H), 1652, 1599(C=C), 1497 (C=N), 1442, 1074, 694; ***m/z found for ($C_{27}H_{20}N_2$):*** 372.4 (M+1).

Anal. Calcd for ***$C_{27}H_{20}N_2$***: C, 87.07; H, 5.41; N, 7.52. Found: C, 87.18; H, 5.36; N, 7.69

1-(4-methoxyphenyl)-2-(2-nitrophenyl)-4,5-diphenyl-1H-imidazole [2j]: M.P.278-280^{o}C

^{1}HNMR (300 MHz, $CDCl_3$): δ 8.28 (s,1H); δ 8.12 (d, 1H); δ 7.88 (d, 1H); δ 7.59 (d, 2H); δ 7.49 (t, 1H); δ 7.26 (m, 9H); δ 7.02 (d, 2H); δ 6.83 (d, 2H); δ 3.79 (s,3H); ***^{13}CNMR (75 MHz, $CDCl_3$):*** 159.79, 148.08, 1144.33, 134.40, 132.18, 131.09, 130.01, 129.92, 129.34, 129.19, 128.53, 128.38, 128.30, 127.36, 127.05, 123.49, 122.89, 114.76, 55.51; ***IR (KBr, cm^{-1}):*** 3057(Ar C-H), 1604(C=C),1527 (C=N), 1442, 1348, 1070, 698; ***m/z found for ($C_{28}H_{21}N_3O_3$):*** 447.1 (M+1)

Anal. Calc. for ***$C_{28}H_{21}N_3O_3$***: C, 75.15; H, 4.73; N, 9.39; O, 10.73. Found: C, 75.23; H, 4.64; N, 9.52; O, 10.88

1,2-bis(4-methoxyphenyl)-4,5-diphenyl-1H-imidazole [2k]: M.P. 158-160^{o}C

^{1}HNMR (300 MHz, $CDCl_3$): δ 7.60 - δ 6.74 (m,18H); δ 3.77 (s, 6H); ***^{13}CNMR (75 MHz, $CDCl_3$):*** 159.54, 159.03, 146.99, 137.73, 134.47, 131.13, 130.78, 130.67, 130.28, 129.92, 129.46, 128.31, 128.12, 127.82, 127.39, 126.49, 56.21; ***IR (KBr, cm^{-1}):*** 3057(Ar C-H), 2935 (Al C-H), 1608(C=C), 1512 (C=N), 1440, 698

m/z found for ($C_{29}H_{24}N_2O_2$): 432.4 (M+1).

Anal. Calcd for ***$C_{29}H_{24}N_2O_2$***: C, 80.53; H, 5.59; N, 6.48; O, 7.40. Found: C, 80.69; H, 5.47; N, 6.54; O, 7.32

4-(1-(4-methoxyphenyl)-4,5-diphenyl-1H-imidazol-2-yl)phenol [2l]: M.P. >280^{o}C

^{1}HNMR (300 MHz, $CDCl_3$): δ 7.65 - δ 6.76 (m, 19H); δ 3.80 (s, 3H); ***^{13}CNMR (75 MHz, $CDCl_3$):*** 160.24, 158.53, 144.99, 137.73, 134.47, 131.13, 130.78, 130.67, 130.28, 129.92, 129.46, 128.31, 128.12, 127.82, 127.79, 116.49, 55.90; ***IR (KBr, cm^{-1}):*** 3037(Ar C-H), 1610(C=C), 1510 (C=N), 1442, 1070, 694; ***m/z found for ($C_{28}H_{22}N_2O_2$):*** 418.6 (M+1).

Anal. Calc. for ***$C_{28}H_{22}N_2O_2$***: C, 80.36; H, 5.30; N, 6.69; O, 7.65. Found: C, 80.39; H, 5.26; N, 6.54; O, 7.55

Imidazole N-oxide

2-(4-methoxyphenyl)-4,5-dimethyl Imidazole N-oxide [3a]: M.P. 138-140 ^{o}C

[1]HNMR (300 MHz, DMSO): δ 8.35 (d, 2H); δ 6.96 (d, 2H); δ 3.77 (s, 1H); δ 2.05 (s, 4H); δ 1.79 (s, 2H): ***[13]CNMR (75 MHz, DMSO):*** 158.43, 127.08, 122.56, 122.06, 113.52, 55.03, 12.15, 7.50; ***IR (KBr, cm^{-1}):*** 3409 (N-H), 3152 (Ar C-H), 2921 (Al C-H), 1614 (C=C), 1507 (C=N), 1384, 1262, 1031; ***m/z found for ($C_{12}H_{14}N_2O_2$):*** 218.2 (M+1)

Anal. Calc. for ***$C_{12}H_{14}N_2O_2$***: C, 66.04; H, 6.47; N, 12.84; O, 14.66. Found: C, 66.21; H, 6.84; N, 12.62; O, 14.80

2-(4-N,N-dimethylphenyl)-4,5-dimethyl Imidazole N-oxide [3b]: M.P. 233-235 °C

[1]HNMR (300 MHz, DMSO): δ 8.01 (d, 2H); δ 7.26(s, 1H); δ 6.48 (d, 2H); δ 2.88 (s, 6H); δ 1.90 (s, 6H): ***[13]CNMR (75 MHz, DMSO):*** 150.54 ; 135.29; 127.73; 124.27; 119.69; 112.32; 111.38; 40.03, 9.56, 7.13; ***IR (KBr, cm^{-1}):*** 3390(N-H), 3050 (Ar C-H), 2921 (Al C-H), 1611 (C=C), 1508 (C=N), 1366, 1205, 1096 cm^{-1}; ***m/z found for ($C_{13}H_{17}N_3O$):*** 232.4 (M+1)

Anal. Calc. for ***$C_{13}H_{17}N_3O$***: C, 67.51; H, 7.41; N, 18.17; O, 6.92. Found: C, 67.22; H, 7.69; N, 18.62; O, 6.54

2-(4-hydroxy phenyl)-4,5-dimethyl Imidazole N-oxide [3c]: M.P. >260 °C

[1]HNMR (300 MHz, DMSO): δ 7.89 (d, 2H); δ 6.77 (d, 2H); δ 2.03 (s, 3H); δ 1.98 (s, 3H): ***[13]CNMR (75 MHz, DMSO):*** 157.18 ; 135.49; 127.21; 123.50; 122.66; 119.36; 114.92; 11.52, 7.28; ***IR (KBr):*** 3409(N-H), 3059 (Ar C-H), 2923 (Al C-H), 1654, 1614 (C=C), 1512 (C=N), 1380, 1286, 1095 cm^{-1}; ***m/z found for ($C_{11}H_{12}N_2O_2$):*** 204.1 (M+1)

Anal. Calc. for ***$C_{11}H_{12}N_2O_2$***: C, 64.69; H, 5.92; N, 13.72; O, 15.67. Found: C, 64.88; H, 5.68; N, 13.62; O, 15.55

2-(3-nitrophenyl)-4,5-dimethyl Imidazole N-oxide [3d]: M.P.172-174 °C

[1]HNMR (300 MHz, DMSO): δ 8.01 (d, 2H); δ 8.81 (s, 1H); δ 8.20 (d, 1H); δ 7.86 (d, 1H); δ 7.50 (d, 1H) δ 1.96 (s, 3H); δ 1.90 (s, 3H);: ***[13]CNMR (75 MHz, DMSO):*** 147.49 ; 130.69; 129.35; 128.78; 127.37; 123.94; 118.84; 118.38, 12.07, 7.27; ***IR (KBr, cm^{-1}):*** 3390(N-H), 3076 (Ar C-H), 2732 (Al C-H), 1646 (C=C), 1523 (C=N), 1347, 1230, 1071 cm^{-1}; ***m/z found for ($C_{11}H_{11}N_3O_3$):*** 233.2 (M+1)

Anal. Calc. for ***$C_{11}H_{11}N_3O_3$***: C, 56.65; H, 4.75; N, 18.02; O, 20.58. Found: C, 56.82; H, 4.68; N, 17.89; O, 20.50

2-(4-hydroxy-3-methoxyphenyl)-4,5-diphenyl Imidazole N-oxide [3e]: M.P.197-199 °C

[1]HNMR (300 MHz, DMSO): δ 9.01 (s, 1H); δ 7.22-7.48 (m, 10H); δ 6.92, δ 6.80, δ 6.62, δ 5.08, δ 3.42 (s, 3H): ***[13]CNMR (75 MHz, DMSO):*** 147.2, 146.7, 145.4, 132.6, 127.9, 127.3, 126.6, 121.1, 118.0, 115.1, 108.9, 55.4; ***IR (KBr, cm^{-1}):*** 3494 (N-H), 3050 (Ar C-H), 2939 (Al C-H), 1600 (C=C), 1496 (C=N), 1267, 1226, 1029; ***m/z found for ($C_{22}H_{18}N_2O_3$):*** 358.1 (M+1)

Anal. Calc. for ***$C_{22}H_{18}N_2O_3$***: C, 73.73; H, 5.06; N, 7.82; O, 13.39. Found: C, 73.56; H, 4.95; N, 7.62; O, 13.58

2-(4-methoxyphenyl)-4,5-diphenyl Imidazole N-oxide [3f]: M.P. 95-96 °C

[1]HNMR (300 MHz, DMSO): δ 9.11 (s, 1H), δ 7.20-7.53 (m, 10H), δ 7.06, δ 6.78, δ 6.32, δ 6.19, δ 5.54, 3.09 (s, 3H); ***[13]CNMR (75 MHz, DMSO):*** 158.93, 145.07, 127.95, 126.73, 126.22, 122.61, 113.61, 54.72; ***IR (KBr,***

cm^{-1}): 3419 (N-H), 3057 (Ar C-H), 2829 (Al C-H), 1608 (C=C), 1494 (C=N), 1298, 1253, 1028, 835, 696; ***m/z found for ($C_{22}H_{18}N_2O_2$):*** 342.4 (M+1)

Anal. Calc. for ***$C_{22}H_{18}N_2O_2$***: C, 77.17; H, 5.30; N, 8.18; O, 9.35. Found: C, 76.98; H, 5.42; N, 8.23; O, 9.32

2-(4-hydroxyphenyl)-4, 5-diphenyl Imidazole N-oxide [3g]: M.P.230-233 ^{o}C

^{1}HNMR (300 MHz, DMSO): δ 8.89 (s, 1H); δ 7.26-7.56 (m, 10H); δ 7.11, δ 6.48, δ 6.32, δ 6.12, δ 5.67 (s, 1H); ***^{13}CNMR (75 MHz, DMSO):*** 158.23 ; 146.53; 135.85; 131.79; 129.04; 128.66; 127.55; 127.32; 126.84; 122.07; 115.86; ***IR (KBr, cm^{-1}):*** 3409 (N-H), 3045 (Ar C-H), 2790 (Al C-H), 1610 (C=C), 1492 (C=N), 1285, 1173, 836, 696; ***m/z found for ($C_{21}H_{16}N_2O_2$):*** 328.1 (M+1)

Anal. Calc. for ***$C_{21}H_{16}N_2O_2$***: C, 76.81; H, 4.91; N, 8.53; O, 9.74. Found: C, 76.88; H, 4.67; N, 8.97; O, 9.65

N-substituted Imidazole-1-oxide

N-butyl-2-(4-hydroxyphenyl)-4,5-dimethyl Imidazole 3-oxide [4a]: M.P. 128-130^{o}C

^{1}HNMR (300 MHz, DMSO): δ 7.45(d, 2H); δ 6.85 (d, 2H); δ 3.84 (t, 2H); δ 2.22 (s, 3H); δ 2.06 (s, 3H) δ 1.43 (m, 2H); δ 1.06 (m, 2H); δ 0.71 (t, 3H): ***^{13}CNMR (75 MHz, DMSO):*** 131.20, 124.16, 119.84, 115.35, 31.59, 18.91, 13.20, 8.53, 7.39; ***IR (KBr, cm^{-1}):*** 3047 (Ar C-H), 2958 (Al C-H), 1602(C=C), 1544(C=N), 1454, 1340, 1282, 1168, 839; ***m/z found for ($C_{15}H_{20}N_2O_2$):*** 260.15 (M+1)

Anal. Calc. for ***$C_{15}H_{20}N_2O_2$***: C, 69.20; H, 7.74; N, 10.76; O, 12.29. Found: C, 69.32; H, 7.84; N, 10.62; O, 12.31

N-napthyl-2-(4-hydroxyphenyl)-4,5-dimethyl Imidazole 3-oxide [4b]:M.P.232-235 ^{o}C

^{1}HNMR (300 MHz, DMSO): δ 6.62 - δ 7.95 (m, 11H); δ 2.00 (t, 6H): ***^{13}CNMR (75 MHz, DMSO):*** 158.50, 138.24, 136.16, 134.25, 131.35, 128.90, 126.50, 126.34, 124.39, 120.25, 116.25, 109.36, 10.87, 5.62; ***IR (KBr, cm^{-1}):*** 3058(Ar C-H), 2925 (Al C-H), 1587(C=C), 1560(C=N), 1510, 1454, 1388, 1245, 1170, 839; ***m/z found for ($C_{21}H_{18}N_2O_2$):*** 330.14 (M+1)

Anal. Calc. for ***$C_{21}H_{18}N_2O_2$***: C, 76.34; H, 5.49; N, 8.48; O, 9.69. Found: C, 76.52; H, 5.36; N, 8.45; O, 9.76

N-(2-nitrophenyl)-2-(4-hydroxyphenyl)-4,5-dimethyl Imidazole 3-oxide [4c]: M.P. 272-273 ^{o}C

^{1}HNMR (300 MHz, $CDCl_3$): δ 8.12 (d, 1H); δ 7.88 (d, 1H); δ 7.59 (d, 2H); δ 7.49 (d, 2H); δ 7.26 (d, 2H); δ 7.02 (d, 2H); δ 4.83 (s, 1H); δ 2.00 (t, 6H); ***^{13}CNMR (75 MHz, $CDCl_3$):*** 159.79, 148.08, 1144.33, 134.40, 132.18, 131.09, 130.01, 129.92, 129.34, 129.19, 128.53, 128.38, 128.30, 127.36, 127.05, 123.49, 122.89, 114.76, 55.51, 10.87, 5.62; ***IR (KBr, cm^{-1}):*** 3200(Ar C-H), 2929 (Al C-H), 1593(C=C), 1510(C=N), 1438, 1350, 1259, 1172, 1105, 837; ***m/z found for ($C_{17}H_{15}N_3O_4$):*** 325.32 (M+1)

Anal. Calc. for ***$C_{17}H_{15}N_3O_4$***: C, 62.76; H, 4.65; N, 12.92; O, 19.67. Found: C, 62.58; H, 4.36; N, 12.85; O, 19.75

N-(4-methoxyphenyl)-2-(4-hydroxyphenyl)-4,5-dimethyl Imidazole 3-oxide [4d]: M.P. 205-207 ^{o}C

[1]HNMR (300 MHz, DMSO): δ 7.20 (d, 2H); δ 6.95 (d, 2H); δ 6.56 (d, 4H); δ 3.73 (s, 3H) δ 2.10 (s, 3H); δ 1.92 (s, 2H); ***[13]CNMR (75 MHz, DMSO):*** 159.15, 130.61, 129.44, 124.67, 115.05, 114.63, 59.79, 55.34, 14.02, 9.08, 7.47; ***IR (KBr, cm^{-1}):*** 3170 (Ar C-H), 2929 (Al C-H), 1608(C=C), 1512(C=N), 1461, 1251,1172, 1031, 833; ***m/z found for ($C_{18}H_{18}N_2O_3$):*** 310.2 (M+1)

Anal. Calc. for ***$C_{18}H_{18}N_2O_3$***: C, 69.66; H, 5.85; N, 9.03; O, 15.47. Found: C, 69.41; H, 5.72; N, 9.21; O, 15.62

1-(4-chlorophenyl)-4,5-diphenyl -1H- Imidazole 3-oxide [4e]: M.P. 170-172°C ***[1]HNMR (300 MHz, DMSO):*** δ 7.42-7.22 (m, 2H); δ 7.12 (t, 2H); ***[13]CNMR (75 MHz, DMSO):*** 136.23, 134.31, 130.53, 129.78, 128.32, 127.94; ***IR (KBr, cm^{-1}):*** 3064 (Ar C-H), 2956 (Al C-H), 1679, 1596 (C=C), 1498 (C=N), 1446, 1367, 1228, 1097, 908; ***m/z found for ($C_{21}H_{15}N_2OCl$):*** 346.1 (M+1)

Anal. Calc. for ***$C_{21}H_{15}N_2OCl$***: C, 72.73; H, 4.36; N, 8.08; O, 4.61; Cl, 10.22. Found: C, 72.65; H, 4.62; N, 8.21; O, 4.81; Cl, 10.28

1-(glycinato)-2-ethyl-4,5-diphenyl Imidazole 3-oxide [4f]: M.P. >260 °C

[1]HNMR (300 MHz, DMSO): δ 10.01 (s, 1H); δ 7.48, δ 7.32, δ 7.13 , δ 4.67, δ 2.87, δ 1.25. ***[13]CNMR (75 MHz, DMSO):*** 169.23, 136.23, 134.31, 130.53, 129.78, 128.32, 127.94, 46.21, 14.62, 13.25; ***IR (KBr, cm^{-1}):*** 3105(Ar C-H), 2952 (Al C-H), 1625, 1595 (C=C), 1498 (C=N), 1436, 1394, 1334, 1126, 1043, 929; ***m/z found for ($C_{19}H_{18}N_2O_3$):*** 322.5 (M+1)

Anal. Calc. for ***$C_{19}H_{18}N_2O_3$***: C, 70.79; H, 5.63; N, 8.69; O, 14.89; Found: C, 70.26; H, 5.58; N, 8.61; O, 14.97

1-(4-chlorophenyl)-2-(4-hydroxyphenyl)-4,5-diphenyl Imidazole 3-oxide [4g]: M.P. 182-184 °C

[1]HNMR (300 MHz, DMSO): δ 7.50 - δ 7.20 (m, ArH); δ 6.65 (d, 2H); ***[13]CNMR (75 MHz, DMSO):*** 157.89, 136.65, 134.13, 130.78, 129.10, 128.94, 127.43, 116.76; ***IR (KBr, cm^{-1}):*** 3057 (Ar C-H), 2885 (Al C-H), 1602, 1573 (C=C), 1485 (C=N), 1442, 1388, 1284, 1161, 1101, 1008, 902, 835; ***m/z found for ($C_{27}H_{19}N_2O_2Cl$):*** 438.7 (M+1)

Anal. Calc. for ***$C_{27}H_{19}N_2O_2Cl$***: C, 73.89; H, 4.36; N, 6.38; O, 7.29; Cl, 8.08. Found: C, 73.77; H, 4.54; N, 6.54; O, 7.45; Cl, 8.15

1-hydroxy Imidazole-3-oxide

1-hydroxy-2-(4-hydroxyphenyl)-4, 5-dimethyl Imidazole 3-oxide [5a]: M.P. 165-168 °C

[1]HNMR (300 MHz, DMSO): δ 7.86 (d, 2H); δ 7.04 (d, 2H); δ 2.27 (s, 6H), δ 2.19 (s, 1H): ***[13]CNMR (75 MHz, DMSO):*** 160.83, 135.26, 131.83, 122.09, 116.06, 110.68, 7.64; ***IR (KBr, cm^{-1}):*** 3400, 3000 (Ar C-H), 2671 (Al C-H), 1611, 1560 (C=C), 1446 (C=N), 1385, 1252, 1178, 1087, 1000, 837 cm^{-1}; ***m/z found for ($C_{11}H_{12}N_2O_3$):*** 220.0 (M+1)

Anal. Calc. for ***$C_{11}H_{12}N_2O_3$***: C, 59.99; H, 5.49; N, 12.72; O, 21.80; Found: C, 60.10; H, 5.32; N, 12.63; O, 21.86

1-hydroxy-2-(4-methoxyphenyl)-4,5-dimethyl Imidazole 3-oxide [5b]: M.P. 196-198 °C

[1]HNMR (300 MHz, DMSO): δ 8.12 (d, 2H); δ 6.93 (d, 2H); δ 3.78 (s, 3H), δ 1.83 (s, 6H): ***[13]CNMR (75 MHz, DMSO):*** 159.10, 129.10, 119.11, 113.21, 55.49, 7.41; ***IR (KBr, cm^{-1}):*** 3418, 3003 (Ar C-H), 2929 (Al C-H),

1610, 1541 (C=C), 1444(C=N), 1380, 1296, 1256, 1182, 1026, 837 cm^{-1}; ***m/z found for ($C_{12}H_{14}N_2O_3$):*** 234.1 (M+1)

Anal. Calc. for ***$C_{12}H_{14}N_2O_3$***: C, 61.53; H, 6.02; N, 11.96; O, 20.49; Found: C, 61.69; H, 6.12; N, 11.87; O, 20.41

1-hydroxy-2-(3-nitrophenyl)-4,5-dimethyl Imidazole 3-oxide [5c]: M.P. 209-211 ^oC

^{1}HNMR (300 MHz, DMSO): δ 9.22 (s, 1H); δ 8.72 (d, 1H); δ 8.05 (d, 1H), δ 7.58 (t, 1H), δ 1.91; ***^{13}CNMR (75 MHz, DMSO):*** 150.20, 134.10, 131.24, 128.21,126.04, 125.12, 121.45, 121.25, 13.49, 5.41; ***IR (KBr, cm^{-1}):*** 3428, 3088 (Ar C-H), 2927 (Al C-H), 2580, 1634, 1530(C=C), 1435(C=N), 1355, 1284, 1248, 812 cm^{-1}; ***m/z found for ($C_{11}H_{11}N_3O_4$):*** 249.1 (M+1)

Anal. Calc. for ***$C_{11}H_{11}N_3O_4$***: C, 53.01; H, 4.45; N, 16.86; O, 25.68; Found: C, 53.39; H, 4.61; N, 16.42; O, 25.54

1-hydroxy-4, 5-dimethyl, 1H Imidazole 3-oxide [5d]: M.P. 136-137 ^oC

^{1}HNMR (300 MHz, DMSO): δ 9.21 (s, 1H); δ 1.96 (s, 6H); ***^{13}CNMR (75 MHz, DMSO):*** 132.25,122.67,115.04, 7.32; ***IR (KBr, cm^{-1}):*** 3300, 3085 (Ar C-H), 2667 (Al C-H), 1886, 1573 (C=C), 1474(C=N), 1404, 1194, 1164, 1091, 997 cm^{-1}; ***m/z found for ($C_5H_8N_2O_2$):*** 128.6 (M+1)

Anal. Calc. for ***$C_5H_8N_2O_2$***: C, 46.87; H, 6.29; N, 21.86; O, 24.97; Found: C, 46.52; H, 6.84; N, 21.25; O, 25.06

1-hydroxy-2-(4-methoxyphenyl)-4,5-diphenyl Imidazole 3-oxide [5e]: M.P. 233-235 ^oC

^{1}HNMR (300 MHz, DMSO): δ 8.82, δ 7.48, δ 7.27, δ 6.90, δ 3.36 (s, 3H); ***^{13}CNMR (75 MHz, DMSO):*** 162.24, 134.10, 133.25, 130.28, 128.14, 127.50, 126.89, 120.90, 120.12, 115.69, 55.49; ***IR (KBr, cm^{-1}):*** 3431, 3055 (Ar C-H), 2835 (Al C-H), 1608, 1575 (C=C), 1488(C=N), 1442, 1394, 1301, 1255, 1087, 1029 cm^{-1}; ***m/z found for ($C_{22}H_{18}N_2O_3$):*** 358.3 (M+1)

Anal. Calc. for ***$C_{22}H_{18}N_2O_3$***: C, 73.73; H, 5.06; N, 7.82; O, 13.39; Found: C, 73.56; H, 4.96; N, 7.65; O, 13.62

Electronic Supporting Information

Appendix I

OUT PUT file of Formaldehyde Monomer via the CBS-QB3 method

Entering Link 1 = C:\G98W\l1.exe PID= 6236.
Copyright (c) 1988,1990,1992,1993,1995,1998 Gaussian, Inc.
All Rights Reserved.
This is part of the Gaussian(R) 98 program. It is based on
the Gaussian 94(TM) system (copyright 1995 Gaussian, Inc.),
the Gaussian 92(TM) system (copyright 1992 Gaussian, Inc.),
the Gaussian 90(TM) system (copyright 1990 Gaussian, Inc.),
the Gaussian 88(TM) system (copyright 1988 Gaussian, Inc.),
the Gaussian 86(TM) system (copyright 1986 Carnegie Mellon
University), and the Gaussian 82(TM) system (copyright 1983
Carnegie Mellon University). Gaussian is a federally registered
trademark of Gaussian, Inc.
This software contains proprietary and confidential information,
including trade secrets, belonging to Gaussian, Inc.
This software is provided under written license and may be
used, copied, transmitted, or stored only in accord with that
written license.
The following legend is applicable only to US Government
contracts under DFARS:

RESTRICTED RIGHTS LEGEND
Use, duplication or disclosure by the US Government is subject
to restrictions as set forth in subparagraph (c)(1)(ii) of the
Rights in Technical Data and Computer Software clause at DFARS
252.227-7013.

Gaussian, Inc.
Carnegie Office Park, Building 6, Pittsburgh, PA 15106 USA

The following legend is applicable only to US Government
contracts under FAR:

RESTRICTED RIGHTS LEGEND

Use, reproduction and disclosure by the US Government is subject
to restrictions as set forth in subparagraph (c) of the
Commercial Computer Software - Restricted Rights clause at FAR
52.227-19.

Gaussian, Inc.
Carnegie Office Park, Building 6, Pittsburgh, PA 15106 USA

Warning -- This program may not be used in any manner that
competes with the business of Gaussian, Inc. or will provide
assistance to any competitor of Gaussian, Inc. The licensee
of this program is prohibited from giving any competitor of
Gaussian, Inc. access to this program. By using this program,
the user acknowledges that Gaussian, Inc. is engaged in the
business of creating and licensing software in the field of
computational chemistry and represents and warrants to the
licensee that it is not a competitor of Gaussian, Inc. and that
it will not use this program in any manner prohibited above.

Cite this work as:
Gaussian 98, Revision A.11.4,
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria,
M. A. Robb, J. R. Cheeseman, V. G. Zakrzewski, J. A. Montgomery, Jr.,
R. E. Stratmann, J. C. Burant, S. Dapprich, J. M. Millam,
A. D. Daniels, K. N. Kudin, M. C. Strain, O. Farkas, J. Tomasi,
V. Barone, M. Cossi, R. Cammi, B. Mennucci, C. Pomelli, C. Adamo,
S. Clifford, J. Ochterski, G. A. Petersson, P. Y. Ayala, Q. Cui,
K. Morokuma, N. Rega, P. Salvador, J. J. Dannenberg, D. K. Malick,
A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. Cioslowski,
J. V. Ortiz, A. G. Baboul, B. B. Stefanov, G. Liu, A. Liashenko,
P. Piskorz, I. Komaromi, R. Gomperts, R. L. Martin, D. J. Fox,
T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe,

P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, J. L. Andres,
C. Gonzalez, M. Head-Gordon, E. S. Replogle, and J. A. Pople,
Gaussian, Inc., Pittsburgh PA, 2002.

****
Gaussian 98: x86-Win32-G98RevA.11.4 7-May-2002
11-Oct-2015
****
%chk=C:\Users\hp\Desktop\1_cbsqb3.chk
Default route: MaxDisk=2000MB
---
opt freq cbs-qb3 geom=connectivity

1/14=-1,18=20,26=3,38=1,57=2/1,3;
2/9=110,17=6,18=5,40=1/2;
3/5=4,6=6,7=700,11=2,25=1,30=1/1,2,3;
4//1;
5/5=2,38=4,42=-5/2;
6/7=2,8=2,9=2,10=2,28=1/1;
7//1,2,3,16;
1/14=-1,18=20/3(1);
99//99;
2/9=110/2;
3/5=4,6=6,7=700,11=2,25=1,30=1/1,2,3;
4/5=5,16=2/1;
5/5=2,38=4,42=-5/2;
7//1,2,3,16;
1/14=-1,18=20/3(-5);
2/9=110/2;
6/7=2,8=2,9=2,10=2,19=2,28=1/1;
99/9=1/99;

Title Card Required

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1
C 0. 0.5449 0.
H -0.67189 1.42372 0.
H 1.08036 0.78339 0.
O -0.41368 -0.58535 0.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Initialization pass.

! Initial Parameters !
! (Angstroms and Degrees) !

! Name Definition Value Derivative Info. !

! R1 R(1,2) 1.1062 estimate D2E/DX2 !
! R2 R(1,3) 1.1064 estimate D2E/DX2 !
! R3 R(1,4) 1.2036 estimate D2E/DX2 !
! A1 A(2,1,3) 114.9503 estimate D2E/DX2 !
! A2 A(2,1,4) 122.498 estimate D2E/DX2 !
! A3 A(3,1,4) 122.5517 estimate D2E/DX2 !
! A4 L(3,1,4,2,-2) 180. estimate D2E/DX2 !

Trust Radius=3.00D-01 FncErr=1.00D-07 GrdErr=1.00D-06
Number of steps in this run= 20 maximum allowed number of steps= 100.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Atomic Atomic Coordinates (Angstroms)
Number Number Type X Y Z
---
1 6 0 0.000000 0.544898 0.000000
2 1 0 -0.671885 1.423719 0.000000
3 1 0 1.080364 0.783394 0.000000
4 8 0 -0.413681 -0.585354 0.000000

Distance matrix (angstroms):
1 2 3 4

```
  1  C   0.000000
  2  H   1.106235  0.000000
  3  H   1.106375  1.865581  0.000000
  4  O   1.203579  2.025597  2.026238  0.000000
Stoichiometry    CH2O
Framework group  CS[SG(CH2O)]
Deg. of freedom    5
Full point group                 CS     NOp   2
Largest Abelian subgroup         CS     NOp   2
Largest concise Abelian subgroup C1     NOp   1
                    Standard orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic           Coordinates (Angstroms)
Number     Number      Type             X           Y           Z
---------------------------------------------------------------------
  1          6           0        0.000027    0.527437    0.000000
  2          1           0       -0.932983    1.121783    0.000000
  3          1           0        0.932598    1.122733    0.000000
  4          8           0        0.000027   -0.676142    0.000000
---------------------------------------------------------------------
Rotational constants (GHZ):    288.1601721     38.8020870     34.1972682
Isotopes: C-12,H-1,H-1,O-16
Standard basis: CBSB7 (5D, 7F)
There are    36 symmetry adapted basis functions of A'  symmetry.
There are    12 symmetry adapted basis functions of A"  symmetry.
Crude estimate of integral set expansion from redundant integrals=1.000.
Integral buffers will be    262144 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
   48 basis functions       80 primitive gaussians
    8 alpha electrons        8 beta electrons
     nuclear repulsion energy       31.3070068345 Hartrees.
One-electron integrals computed using PRISM.
NBasis=    48 RedAO= T  NBF=    36    12
NBsUse=    48 1.00D-04 NBFU=    36    12
Projected INDO Guess.
Initial guess orbital symmetries:
     Occupied  (A') (A') (A') (A') (A') (A') (A") (A')
     Virtual   (A") (A') (A') (A') (A') (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A') (A') (A') (A')
               (A") (A") (A") (A") (A") (A") (A") (A") (A")
Requested convergence on RMS density matrix=1.00D-08 within  64 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Keep R1 and R2 integrals in memory in canonical form, NReq=     2069797.
Integral accuracy reduced to 1.0D-05 until final iterations.
Initial convergence to 1.0D-05 achieved.  Increase integral accuracy.
SCF Done:  E(RB+HF-LYP) =  -114.536296127     A.U. after   12 cycles
          Convg  =    0.7987D-08           -V/T =  2.0031
          S**2   =   0.0000

**********************************************************************

        Population analysis using the SCF density.

**********************************************************************

Orbital Symmetries:
     Occupied  (A') (A') (A') (A') (A') (A') (A") (A')
     Virtual   (A") (A') (A') (A') (A') (A") (A') (A') (A') (A')
               (A') (A") (A') (A") (A") (A') (A') (A') (A') (A')
               (A") (A") (A') (A') (A') (A') (A') (A") (A") (A')
               (A") (A') (A') (A') (A') (A") (A') (A') (A') (A')
 The electronic state is 1-A'.
Alpha  occ. eigenvalues --  -19.13768 -10.27082  -1.06654  -0.64016  -0.49959
Alpha  occ. eigenvalues --   -0.45620  -0.40567  -0.27309
Alpha virt. eigenvalues --   -0.05042   0.04882   0.10542   0.18544   0.31424
Alpha virt. eigenvalues --    0.38383   0.39414   0.53540   0.59454   0.63107
Alpha virt. eigenvalues --    0.74342   0.82947   0.91581   1.00689   1.25191
Alpha virt. eigenvalues --    1.28074   1.38755   1.39796   1.57181   1.60277
Alpha virt. eigenvalues --    1.74018   1.83593   2.08165   2.28240   2.39591
Alpha virt. eigenvalues --    2.41326   2.53000   2.56076   2.86855   2.88313
Alpha virt. eigenvalues --    3.30215   3.33596   3.42259   3.69591   3.77575
Alpha virt. eigenvalues --    4.82148   4.94112   5.50427  23.84588  49.88999
```

```
      Condensed to atoms (all electrons):
               1          2          3          4
 1  C    4.583461   0.364776   0.364676   0.586904
 2  H    0.364776   0.713481  -0.101656  -0.053002
 3  H    0.364676  -0.101656   0.713512  -0.052923
 4  O    0.586904  -0.053002  -0.052923   7.771999
Total atomic charges:
               1
 1  C    0.100184
 2  H    0.076402
 3  H    0.076392
 4  O   -0.252978
Sum of Mulliken charges=   0.00000
Atomic charges with hydrogens summed into heavy atoms:
               1
 1  C    0.252978
 2  H    0.000000
 3  H    0.000000
 4  O   -0.252978
Sum of Mulliken charges=   0.00000
Electronic spatial extent (au):  <R**2>=    60.3793
Charge=     0.0000 electrons
Dipole moment (Debye):
   X=     0.0000    Y=     2.2616    Z=     0.0000  Tot=     2.2616
Quadrupole moment (Debye-Ang):
  XX=   -11.5902   YY=   -12.0437   ZZ=   -11.5370
  XY=     0.0007   XZ=     0.0000   YZ=     0.0000
Octapole moment (Debye-Ang**2):
 XXX=    -0.0009  YYY=    -0.9646  ZZZ=     0.0000  XYY=     0.0012
 XXY=     0.0602  XXZ=     0.0000  XZZ=     0.0000  YZZ=    -0.9224
 YYZ=     0.0000  XYZ=     0.0000
Hexadecapole moment (Debye-Ang**3):
XXXX=   -18.4729 YYYY=   -44.9310 ZZZZ=    -9.8129 XXXY=    -0.0011
XXXZ=     0.0000 YYYX=     0.0015 YYYZ=     0.0000 ZZZX=     0.0000
ZZZY=     0.0000 XXYY=   -10.1537 XXZZ=    -4.9694 YYZZ=    -9.1173
XXYZ=     0.0000 YYXZ=     0.0000 ZZXY=    -0.0004
N-N= 3.130700683453D+01 E-N=-3.318076813691D+02  KE= 1.141854217237D+02
Symmetry A'   KE= 1.105024792481D+02
Symmetry A"   KE= 3.682942475637D+00
***** Axes restored to original set *****
-------------------------------------------------------------------
Center     Atomic                Forces (Hartrees/Bohr)
Number     Number           X            Y            Z
-------------------------------------------------------------------
   1        6        -0.002185537   -0.005830470    0.000000000
   2        1        -0.002087284    0.000936505    0.000000000
   3        1         0.002129022   -0.000733487    0.000000000
   4        8         0.002143798    0.005627452    0.000000000
-------------------------------------------------------------------
Cartesian Forces:  Max     0.005830470 RMS     0.002666764

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Internal  Forces:  Max     0.006021449 RMS     0.002611688
Search for a local minimum.
Step number   1 out of a maximum of  20
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Second derivative matrix not updated -- first step.
The second derivative matrix:
                R1       R2       R3       A1       A2
       R1        0.33002
       R2        0.00000   0.32987
       R3        0.00000   0.00000   1.03045
       A1        0.00000   0.00000   0.00000   0.16000
       A2        0.00000   0.00000   0.00000   0.00000   0.16000
       A3        0.00000   0.00000   0.00000   0.00000   0.00000
       A4        0.00000   0.00000   0.00000   0.00000   0.00000
                A3       A4
       A3        0.16000
       A4        0.00000   0.16000
   Eigenvalues ---    0.16000   0.16000   0.16000   0.32987   0.33002
   Eigenvalues ---    1.030451000.00000
RFO step:  Lambda=-8.20630066D-05.
Linear search not attempted -- first point.
```

```
Iteration  1 RMS(Cart)=  0.00667331 RMS(Int)=  0.00001882
Iteration  2 RMS(Cart)=  0.00001489 RMS(Int)=  0.00000000
Iteration  3 RMS(Cart)=  0.00000000 RMS(Int)=  0.00000000
Variable      Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                        (Linear)    (Quad)   (Total)
  R1       2.09048   0.00201   0.00000   0.00609   0.00609   2.09658
  R2       2.09075   0.00192   0.00000   0.00582   0.00582   2.09657
  R3       2.27443  -0.00602   0.00000  -0.00584  -0.00584   2.26859
  A1       2.00626   0.00158   0.00000   0.00986   0.00986   2.01612
  A2       2.13799  -0.00070   0.00000  -0.00437  -0.00437   2.13363
  A3       2.13893  -0.00088   0.00000  -0.00549  -0.00549   2.13344
  A4       3.14159   0.00000   0.00000   0.00000   0.00000   3.14159
     Item               Value     Threshold  Converged?
Maximum Force            0.006021     0.000450     NO
RMS     Force            0.002612     0.000300     NO
Maximum Displacement     0.011349     0.001800     NO
RMS     Displacement     0.006678     0.001200     NO
Predicted change in Energy=-4.102118D-05
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

                         Input orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic           Coordinates (Angstroms)
Number     Number      Type             X           Y           Z
---------------------------------------------------------------------
  1          6           0        0.181418    0.495988    0.000000
  2          1           0       -0.496580    1.374179    0.000000
  3          1           0        1.266004    0.729580    0.000000
  4          8           0       -0.230801   -0.631507    0.000000
---------------------------------------------------------------------
                Distance matrix (angstroms):
                     1          2          3          4
   1  C    0.000000
   2  H    1.109460   0.000000
   3  H    1.109456   1.876756   0.000000
   4  O    1.200487   2.023219   2.023113   0.000000
Stoichiometry    CH2O
Framework group  CS[SG(CH2O)]
Deg. of freedom    5
Full point group                 CS     NOp   2
Largest Abelian subgroup         CS     NOp   2
Largest concise Abelian subgroup C1     NOp   1
                         Standard orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic           Coordinates (Angstroms)
Number     Number      Type             X           Y           Z
---------------------------------------------------------------------
  1          6           0        0.000007    0.526256    0.000000
  2          1           0        0.938331    1.118242    0.000000
  3          1           0       -0.938424    1.118067    0.000000
  4          8           0        0.000007   -0.674231    0.000000
---------------------------------------------------------------------
Rotational constants (GHZ):    284.7388319     39.0224208     34.3191115
Isotopes: C-12,H-1,H-1,O-16
Standard basis: CBSB7 (5D, 7F)
There are    36 symmetry adapted basis functions of A'  symmetry.
There are    12 symmetry adapted basis functions of A"  symmetry.
Crude estimate of integral set expansion from redundant integrals=1.000.
Integral buffers will be    262144 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
   48 basis functions       80 primitive gaussians
    8 alpha electrons        8 beta electrons
      nuclear repulsion energy       31.3490477358 Hartrees.
One-electron integrals computed using PRISM.
NBasis=    48 RedAO= T  NBF=    36    12
NBsUse=    48 1.00D-04 NBFU=    36    12
Initial guess read from the read-write file:
Initial guess orbital symmetries:
     Occupied  (A') (A') (A') (A') (A') (A') (A") (A')
     Virtual   (A") (A') (A') (A') (A') (A") (A') (A') (A') (A')
               (A') (A") (A') (A") (A") (A') (A') (A') (A') (A')
               (A") (A") (A') (A') (A') (A') (A') (A") (A") (A')
               (A") (A') (A') (A') (A') (A") (A') (A') (A') (A')
```

Requested convergence on RMS density matrix=1.00D-08 within 64 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Keep R1 and R2 integrals in memory in canonical form, NReq= 2069797.
SCF Done: E(RB+HF-LYP) = -114.536340751 A.U. after 10 cycles
Convg = 0.4427D-08 -V/T = 2.0030
S**2 = 0.0000
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000352655	-0.001024670	0.000000000
2	1	-0.000132838	0.000180660	0.000000000
3	1	0.000218864	0.000069651	0.000000000
4	8	0.000266629	0.000774359	0.000000000

Cartesian Forces: Max 0.001024670 RMS 0.000402914

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Internal Forces: Max 0.000818831 RMS 0.000332559
Search for a local minimum.
Step number 2 out of a maximum of 20
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Update second derivatives using information from points 1 2
Trust test= 1.09D+00 RLast= 1.59D-02 DXMaxT set to 3.00D-01
The second derivative matrix:

	R1	R2	R3	A1	A2
R1	0.32339				
R2	-0.00668	0.32316			
R3	0.02341	0.02336	0.95004		
A1	-0.00054	-0.00083	0.00479	0.16374	
A2	0.00063	0.00074	-0.00327	-0.00131	0.16043
A3	-0.00009	0.00009	-0.00152	-0.00244	0.00088
A4	0.00000	0.00000	0.00000	0.00000	0.00000

	A3	A4
A3	0.16156	
A4	0.00000	0.16000

Eigenvalues --- 0.15993 0.16000 0.16573 0.31489 0.32996
Eigenvalues --- 0.951811000.00000
RFO step: Lambda=-4.08972494D-07.
Quartic linear search produced a step of 0.09587.
Iteration 1 RMS(Cart)= 0.00041264 RMS(Int)= 0.00000002
Iteration 2 RMS(Cart)= 0.00000002 RMS(Int)= 0.00000000

Variable	Old X	-DE/DX (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.09658	0.00022	0.00058	0.00019	0.00077	2.09735
R2	2.09657	0.00023	0.00056	0.00023	0.00079	2.09736
R3	2.26859	-0.00082	-0.00056	-0.00034	-0.00090	2.26769
A1	2.01612	-0.00002	0.00095	-0.00103	-0.00008	2.01604
A2	2.13363	-0.00001	-0.00042	0.00034	-0.00008	2.13355
A3	2.13344	0.00003	-0.00053	0.00068	0.00016	2.13360
A4	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159

Item	Value	Threshold	Converged?
Maximum Force	0.000819	0.000450	NO
RMS Force	0.000333	0.000300	NO
Maximum Displacement	0.000632	0.001800	YES
RMS Displacement	0.000413	0.001200	YES

Predicted change in Energy=-5.485780D-07
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.180644	0.494016	0.000000
2	1	0	-0.497607	1.372530	0.000000
3	1	0	1.265618	0.727787	0.000000
4	8	0	-0.231495	-0.633001	0.000000

Distance matrix (angstroms):

	1	2	3	4
1 C	0.000000			

```
   2  H    1.109870   0.000000
   3  H    1.109873   1.877406   0.000000
   4  O    1.200010   2.023109   2.023140   0.000000
Stoichiometry    CH2O
Framework group  CS[SG(CH2O)]
Deg. of freedom    5
Full point group                 CS     NOp   2
Largest Abelian subgroup         CS     NOp   2
Largest concise Abelian subgroup C1     NOp   1
                     Standard orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic           Coordinates (Angstroms)
Number     Number      Type             X           Y           Z
---------------------------------------------------------------------
  1          6           0        0.000002    0.525985    0.000000
  2          1           0       -0.938715    1.118119    0.000000
  3          1           0        0.938691    1.118168    0.000000
  4          8           0        0.000002   -0.674025    0.000000
---------------------------------------------------------------------
Rotational constants (GHZ):    284.5414197     39.0462381     34.3346594
Isotopes: C-12,H-1,H-1,O-16
Standard basis: CBSB7 (5D, 7F)
There are    36 symmetry adapted basis functions of A'  symmetry.
There are    12 symmetry adapted basis functions of A"  symmetry.
Crude estimate of integral set expansion from redundant integrals=1.000.
Integral buffers will be    262144 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
   48 basis functions       80 primitive gaussians
    8 alpha electrons        8 beta electrons
      nuclear repulsion energy       31.3552993902 Hartrees.
One-electron integrals computed using PRISM.
NBasis=    48 RedAO= T  NBF=    36    12
NBsUse=    48 1.00D-04 NBFU=    36    12
Initial guess read from the read-write file:
Initial guess orbital symmetries:
     Occupied  (A') (A') (A') (A') (A') (A') (A") (A')
     Virtual   (A") (A') (A') (A') (A') (A") (A') (A') (A') (A')
               (A') (A") (A') (A") (A") (A') (A') (A') (A') (A')
               (A") (A") (A') (A') (A') (A') (A') (A") (A") (A')
               (A") (A') (A') (A') (A') (A") (A') (A') (A') (A')
Requested convergence on RMS density matrix=1.00D-08 within  64 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Keep R1 and R2 integrals in memory in canonical form, NReq=     2069797.
SCF Done:  E(RB+HF-LYP) =  -114.536341361     A.U. after   10 cycles
          Convg  =    0.4375D-08           -V/T =  2.0030
          S**2   =   0.0000
***** Axes restored to original set *****
---------------------------------------------------------------------
Center     Atomic                 Forces (Hartrees/Bohr)
Number     Number           X              Y              Z
---------------------------------------------------------------------
  1          6       -0.000066244   -0.000168030    0.000000000
  2          1        0.000017523    0.000046143    0.000000000
  3          1        0.000014803    0.000041519    0.000000000
  4          8        0.000033919    0.000080369    0.000000000
---------------------------------------------------------------------
Cartesian Forces:  Max     0.000168030 RMS     0.000060972

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Internal  Forces:  Max     0.000087129 RMS     0.000043886
Search for a local minimum.
Step number   3 out of a maximum of  20
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Update second derivatives using information from points  1  2  3
Trust test= 1.11D+00 RLast= 1.44D-03 DXMaxT set to 3.00D-01
The second derivative matrix:
                R1       R2       R3       A1       A2
       R1        0.31796
       R2       -0.01158   0.31883
       R3        0.04177   0.03977   0.88819
       A1        0.01099   0.01102  -0.03690   0.16689
       A2       -0.00612  -0.00625   0.02125  -0.00402   0.16255
```

```
        A3       -0.00486  -0.00477   0.01565  -0.00287   0.00147
        A4        0.00000   0.00000   0.00000   0.00000   0.00000
                  A3        A4
        A3        0.16140
        A4        0.00000   0.16000
     Eigenvalues ---    0.16000   0.16040   0.16387   0.30513   0.32998
     Eigenvalues ---    0.896441000.00000
RFO step:  Lambda=-3.30785868D-08.
Quartic linear search produced a step of  0.12553.
Iteration  1 RMS(Cart)=  0.00014125 RMS(Int)=  0.00000002
Iteration  2 RMS(Cart)=  0.00000002 RMS(Int)=  0.00000000
Variable      Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                       (Linear)    (Quad)   (Total)
   R1       2.09735   0.00003   0.00010   0.00002   0.00012   2.09747
   R2       2.09736   0.00002   0.00010   0.00001   0.00011   2.09747
   R3       2.26769  -0.00009  -0.00011  -0.00002  -0.00013   2.26756
   A1       2.01604  -0.00006  -0.00001  -0.00036  -0.00037   2.01567
   A2       2.13355   0.00003  -0.00001   0.00023   0.00022   2.13377
   A3       2.13360   0.00002   0.00002   0.00013   0.00015   2.13375
   A4       3.14159   0.00000   0.00000   0.00000   0.00000   3.14159
       Item               Value     Threshold  Converged?
Maximum Force            0.000087     0.000450     YES
RMS     Force            0.000044     0.000300     YES
Maximum Displacement     0.000209     0.001800     YES
RMS     Displacement     0.000141     0.001200     YES
Predicted change in Energy=-2.421932D-08
Optimization completed.
   -- Stationary point found.
                          ----------------------------
                          !   Optimized Parameters   !
                          ! (Angstroms and Degrees)  !
--------------------------                          --------------------------
! Name  Definition              Value          Derivative Info.            !
--------------------------------------------------------------------------------
! R1    R(1,2)                  1.1099         -DE/DX =    0.              !
! R2    R(1,3)                  1.1099         -DE/DX =    0.              !
! R3    R(1,4)                  1.2            -DE/DX =   -0.0001          !
! A1    A(2,1,3)                115.5104         -DE/DX =   -0.0001          !
! A2    A(2,1,4)                122.2433         -DE/DX =    0.              !
! A3    A(3,1,4)                122.2462         -DE/DX =    0.              !
! A4    L(3,1,4,2,-2)           180.           -DE/DX =    0.              !
--------------------------------------------------------------------------------
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

                         Input orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic           Coordinates (Angstroms)
Number     Number      Type             X           Y           Z
---------------------------------------------------------------------
    1          6           0        0.180649    0.493990    0.000000
    2          1           0       -0.497601    1.372505    0.000000
    3          1           0        1.265624    0.727762    0.000000
    4          8           0       -0.231490   -0.633026    0.000000
---------------------------------------------------------------------
                  Distance matrix (angstroms):
                       1        2        3        4
     1  C    0.000000
     2  H    1.109870   0.000000
     3  H    1.109873   1.877406   0.000000
     4  O    1.200010   2.023109   2.023140   0.000000
Stoichiometry    CH2O
Framework group  CS[SG(CH2O)]
Deg. of freedom    5
Full point group                 CS     NOp   2
Largest Abelian subgroup         CS     NOp   2
Largest concise Abelian subgroup C1     NOp   1
                         Standard orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic           Coordinates (Angstroms)
Number     Number      Type             X           Y           Z
---------------------------------------------------------------------
    1          6           0        0.000002    0.525985    0.000000
    2          1           0       -0.938715    1.118119    0.000000
    3          1           0        0.938691    1.118168    0.000000
```

```
  4        8           0       0.000002   -0.674025    0.000000
---------------------------------------------------------------------
Rotational constants (GHZ):    284.5414197     39.0462381     34.3346594
Isotopes: C-12,H-1,H-1,O-16

*********************************************************************

        Population analysis using the SCF density.

*********************************************************************

Orbital Symmetries:
     Occupied  (A') (A') (A') (A') (A') (A') (A") (A')
     Virtual   (A") (A') (A') (A') (A') (A") (A') (A') (A') (A')
               (A') (A") (A') (A") (A") (A') (A') (A') (A') (A')
               (A") (A") (A') (A') (A') (A') (A') (A") (A") (A')
               (A") (A') (A') (A') (A') (A") (A') (A') (A') (A')
 The electronic state is 1-A'.
Alpha  occ. eigenvalues --  -19.13742 -10.27087  -1.06856  -0.63826  -0.50015
Alpha  occ. eigenvalues --   -0.45639  -0.40686  -0.27281
Alpha virt. eigenvalues --   -0.04932   0.04842   0.10518   0.18608   0.31171
Alpha virt. eigenvalues --    0.38362   0.39574   0.53424   0.59554   0.63350
Alpha virt. eigenvalues --    0.74315   0.82955   0.91614   1.00587   1.25421
Alpha virt. eigenvalues --    1.28176   1.38691   1.39282   1.57389   1.60594
Alpha virt. eigenvalues --    1.73568   1.83555   2.07565   2.28376   2.39199
Alpha virt. eigenvalues --    2.41080   2.52752   2.56034   2.86910   2.88362
Alpha virt. eigenvalues --    3.30529   3.34263   3.42838   3.68698   3.77269
Alpha virt. eigenvalues --    4.82223   4.94220   5.50749  23.84521  49.89334
       Condensed to atoms (all electrons):
             1        2        3        4
 1  C    4.583056   0.363892   0.363887   0.589094
 2  H    0.363892   0.715157  -0.100924  -0.053672
 3  H    0.363887  -0.100924   0.715158  -0.053667
 4  O    0.589094  -0.053672  -0.053667   7.769410
Total atomic charges:
             1
 1  C    0.100071
 2  H    0.075547
 3  H    0.075548
 4  O   -0.251165
Sum of Mulliken charges=   0.00000
Atomic charges with hydrogens summed into heavy atoms:
             1
 1  C    0.251165
 2  H    0.000000
 3  H    0.000000
 4  O   -0.251165
Sum of Mulliken charges=   0.00000
Electronic spatial extent (au):  <R**2>=    60.2927
Charge=     0.0000 electrons
Dipole moment (Debye):
   X=     0.0000    Y=     2.2401    Z=     0.0000  Tot=     2.2401
Quadrupole moment (Debye-Ang):
  XX=   -11.5794   YY=   -12.0741   ZZ=   -11.5371
  XY=     0.0000   XZ=     0.0000   YZ=     0.0000
Octapole moment (Debye-Ang**2):
 XXX=     0.0000  YYY=    -1.0421  ZZZ=     0.0000  XYY=     0.0001
 XXY=     0.0506  XXZ=     0.0000  XZZ=     0.0000  YZZ=    -0.9333
 YYZ=     0.0000  XYZ=     0.0000
Hexadecapole moment (Debye-Ang**3):
XXXX=   -18.5892 YYYY=   -44.8588 ZZZZ=    -9.8116 XXXY=     0.0000
XXXZ=     0.0000 YYYX=     0.0001 YYYZ=     0.0000 ZZZX=     0.0000
ZZZY=     0.0000 XXYY=   -10.1562 XXZZ=    -4.9945 YYZZ=    -9.0953
XXYZ=     0.0000 YYXZ=     0.0000 ZZXY=     0.0000
N-N= 3.135529939020D+01 E-N=-3.319060213454D+02  KE= 1.141905271353D+02
Symmetry A'   KE= 1.105048084021D+02
Symmetry A"   KE= 3.685718733203D+00
1|1|UNPC-UNK|FOpt|RB3LYP|CBSB7|C1H2O1|PCUSER|11-Oct-2015|0||# OPT FREQ
 CBS-QB3 GEOM=CONNECTIVITY||Title Card Required||0,1|C,0.1806494346,0.
4939903678,0.|H,-0.497601017,1.3725046282,0.|H,1.2656239041,0.72776214
71,0.|O,-0.2314899368,-0.6330261227,0.||Version=x86-Win32-G98RevA.11.4
|State=1-A'|HF=-114.5363414|RMSD=4.375e-009|RMSF=6.097e-005|Dipole=0.3
026799,0.8276897,0.|PG=CS [SG(C1H2O1)]||@
```

TO SEE A WORLD IN A GRAIN OF SAND
AND A HEAVEN IN A WILD FLOWER
HOLD INFINITY IN THE PALM OF YOUR HAND
AND ETERNITY IN AN HOUR

-- WILLIAM BLAKE

Job cpu time: 0 days 0 hours 0 minutes 21.0 seconds.
File lengths (MBytes): RWF= 6 Int= 0 D2E= 0 Chk= 3 Scr= 1
Normal termination of Gaussian 98.
Link1: Proceeding to internal job step number 2.

#N Geom=AllCheck Guess=TCheck B3LYP/CBSB7 Freq

1/10=4,29=7,30=1,38=1/1,3;
2/40=1/2;
3/5=4,6=6,7=700,11=2,25=1,30=1/1,2,3;
4/5=101/1;
5/5=2,42=-5/2;
8/6=4,11=11,23=2,27=262144000/1;
11/6=1,8=1,9=11,15=111,16=11/1,2,10;
10/6=1/2;
6/7=2,8=2,9=2,10=2,18=1,28=1/1;
7/8=1,10=1,25=1/1,2,3,16;
1/10=4,30=1/3;
99//99;

Title Card Required

Redundant internal coordinates taken from checkpoint file:
C:\Users\hp\Desktop\1_cbsqb3.chk
Charge = 0 Multiplicity = 1
C,0,0.1806494346,0.4939903678,0.
H,0,-0.497601017,1.3725046282,0.
H,0,1.2656239041,0.7277621471,0.
O,0,-0.2314899368,-0.6330261227,0.
Recover connectivity data from disk.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Initialization pass.

! Initial Parameters !
! (Angstroms and Degrees) !

! Name	Definition	Value	Derivative Info.
! R1	R(1,2)	1.1099	calculate D2E/DX2 analytically!
! R2	R(1,3)	1.1099	calculate D2E/DX2 analytically!
! R3	R(1,4)	1.2	calculate D2E/DX2 analytically!
! A1	A(2,1,3)	115.5104	calculate D2E/DX2 analytically!
! A2	A(2,1,4)	122.2433	calculate D2E/DX2 analytically!
! A3	A(3,1,4)	122.2462	calculate D2E/DX2 analytically!
! A4	L(3,1,4,2,-2)	180.	calculate D2E/DX2 analytically!

Trust Radius=3.00D-01 FncErr=1.00D-07 GrdErr=1.00D-07
Number of steps in this run= 20 maximum allowed number of steps= 100.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.180649	0.493990	0.000000
2	1	0	-0.497601	1.372505	0.000000
3	1	0	1.265624	0.727762	0.000000
4	8	0	-0.231490	-0.633026	0.000000

Distance matrix (angstroms):

		1	2	3	4
1	C	0.000000			
2	H	1.109870	0.000000		
3	H	1.109873	1.877406	0.000000	

```
  4 O    1.200010   2.023109   2.023140   0.000000
                Interatomic angles:
   H2-C1-H3=115.5104      H2-C1-O4=122.2433      H3-C1-O4=122.2462
   H3-H2-O4= 62.3562
Stoichiometry    CH2O
Framework group  CS[SG(CH2O)]
Deg. of freedom    5
Full point group              CS     NOp   2
Largest Abelian subgroup      CS     NOp   2
Largest concise Abelian subgroup C1     NOp   1
                Standard orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic           Coordinates (Angstroms)
Number     Number      Type             X         Y         Z
---------------------------------------------------------------------
  1        6           0        0.000002    0.525985    0.000000
  2        1           0       -0.938715    1.118119    0.000000
  3        1           0        0.938691    1.118168    0.000000
  4        8           0        0.000002   -0.674025    0.000000
---------------------------------------------------------------------
Rotational constants (GHZ):    284.5414197     39.0462381     34.3346594
Isotopes: C-12,H-1,H-1,O-16
Standard basis: CBSB7 (5D, 7F)
There are    36 symmetry adapted basis functions of A'  symmetry.
There are    12 symmetry adapted basis functions of A"  symmetry.
Crude estimate of integral set expansion from redundant integrals=1.000.
Integral buffers will be    262144 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
   48 basis functions       80 primitive gaussians
    8 alpha electrons       8 beta electrons
     nuclear repulsion energy       31.3552993902 Hartrees.
One-electron integrals computed using PRISM.
NBasis=    48 RedAO= T  NBF=    36    12
NBsUse=    48 1.00D-04 NBFU=    36    12
Initial guess read from the checkpoint file:
C:\Users\hp\Desktop\1_cbsqb3.chk
Initial guess orbital symmetries:
     Occupied  (A') (A') (A') (A') (A') (A') (A") (A')
     Virtual   (A") (A') (A') (A') (A') (A") (A') (A') (A') (A')
               (A') (A") (A') (A") (A") (A') (A') (A') (A') (A')
               (A") (A") (A') (A') (A') (A') (A') (A") (A") (A')
               (A") (A') (A') (A') (A') (A") (A') (A') (A') (A')
Requested convergence on RMS density matrix=1.00D-08 within  64 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Keep R1 and R2 integrals in memory in canonical form, NReq=     2069797.
SCF Done:  E(RB+HF-LYP) =  -114.536341361     A.U. after    1 cycles
          Convg  =    0.2220D-08           -V/T =  2.0030
          S**2   =   0.0000
Range of M.O.s used for correlation:     1    48
NBasis=    48 NAE=     8 NBE=     8 NFC=     0 NFV=     0
NROrb=     48 NOA=     8 NOB=     8 NVA=    40 NVB=    40
G2DrvN: will do    4 atoms at a time, making    1 passes doing MaxLOS=2.
FoFDir used for L=0 through L=2.
       Differentiating once with respect to electric field.
          with respect to dipole field.
       Differentiating once with respect to nuclear coordinates.
       Store integrals in memory, NReq=     2067158.
       There are  15 degrees of freedom in the 1st order CPHF.
 12 vectors were produced by pass  0.
AX will form  12 AO Fock derivatives at one time.
 12 vectors were produced by pass  1.
 12 vectors were produced by pass  2.
 12 vectors were produced by pass  3.
 12 vectors were produced by pass  4.
 10 vectors were produced by pass  5.
  1 vectors were produced by pass  6.
Inv2:  IOpt= 1 Iter= 1 AM= 1.39D-15 Conv= 1.00D-12.
Inverted reduced A of dimension  71 with in-core refinement.

*******************************************************************

        Population analysis using the SCF density.
```

```
**********************************************************************

Orbital Symmetries:
     Occupied  (A') (A') (A') (A') (A') (A') (A") (A')
     Virtual   (A") (A') (A') (A') (A') (A") (A') (A') (A') (A')
               (A') (A") (A') (A") (A") (A') (A') (A') (A') (A')
               (A") (A") (A') (A') (A') (A') (A') (A") (A") (A')
               (A") (A') (A') (A') (A') (A") (A') (A') (A') (A')
 The electronic state is 1-A'.
Alpha  occ. eigenvalues --  -19.13742 -10.27087  -1.06856  -0.63826  -0.50015
Alpha  occ. eigenvalues --   -0.45639  -0.40686  -0.27281
Alpha virt. eigenvalues --   -0.04932   0.04842   0.10518   0.18608   0.31171
Alpha virt. eigenvalues --    0.38362   0.39574   0.53424   0.59554   0.63350
Alpha virt. eigenvalues --    0.74315   0.82955   0.91614   1.00587   1.25421
Alpha virt. eigenvalues --    1.28176   1.38691   1.39282   1.57389   1.60594
Alpha virt. eigenvalues --    1.73568   1.83555   2.07565   2.28376   2.39199
Alpha virt. eigenvalues --    2.41080   2.52752   2.56034   2.86910   2.88362
Alpha virt. eigenvalues --    3.30529   3.34263   3.42838   3.68698   3.77269
Alpha virt. eigenvalues --    4.82223   4.94220   5.50749  23.84521  49.89334
          Condensed to atoms (all electrons):
               1          2          3          4
 1  C    4.583056   0.363892   0.363887   0.589094
 2  H    0.363892   0.715157  -0.100924  -0.053672
 3  H    0.363887  -0.100924   0.715158  -0.053667
 4  O    0.589094  -0.053672  -0.053667   7.769410
Total atomic charges:
               1
 1  C    0.100071
 2  H    0.075547
 3  H    0.075548
 4  O   -0.251165
Sum of Mulliken charges=   0.00000
Atomic charges with hydrogens summed into heavy atoms:
               1
 1  C    0.251165
 2  H    0.000000
 3  H    0.000000
 4  O   -0.251165
Sum of Mulliken charges=   0.00000
Electronic spatial extent (au):  <R**2>=    60.2927
Charge=     0.0000 electrons
Dipole moment (Debye):
   X=     0.0000    Y=     2.2401    Z=     0.0000  Tot=     2.2401
Quadrupole moment (Debye-Ang):
  XX=   -11.5794   YY=   -12.0741   ZZ=   -11.5371
  XY=     0.0000   XZ=     0.0000   YZ=     0.0000
Octapole moment (Debye-Ang**2):
 XXX=     0.0000  YYY=    -1.0421  ZZZ=     0.0000  XYY=     0.0001
 XXY=     0.0506  XXZ=     0.0000  XZZ=     0.0000  YZZ=    -0.9333
 YYZ=     0.0000  XYZ=     0.0000
Hexadecapole moment (Debye-Ang**3):
XXXX=   -18.5892 YYYY=   -44.8588 ZZZZ=    -9.8116 XXXY=     0.0000
XXXZ=     0.0000 YYYX=     0.0001 YYYZ=     0.0000 ZZZX=     0.0000
ZZZY=     0.0000 XXYY=   -10.1562 XXZZ=    -4.9945 YYZZ=    -9.0953
XXYZ=     0.0000 YYXZ=     0.0000 ZZXY=     0.0000
N-N= 3.135529939020D+01 E-N=-3.319060225326D+02  KE= 1.141905277053D+02
Symmetry A'   KE= 1.105048087173D+02
Symmetry A"   KE= 3.685718988055D+00
 Exact polarizability:  14.438   0.000  19.186   0.000   0.000   7.929
Approx polarizability:  16.974   0.000  31.496   0.000   0.000  10.356
Full mass-weighted force constant matrix:
Low frequencies ---  -16.3626  -10.6605   -0.0005    0.0010    0.0018   12.3195
Low frequencies --- 1201.9929 1270.1599 1538.9564
Harmonic frequencies (cm**-1), IR intensities (KM/Mole),
Raman scattering activities (A**4/AMU), Raman depolarization ratios,
reduced masses (AMU), force constants (mDyne/A) and normal coordinates:
                 1                 2                 3
                A"                A'                A'
Frequencies --  1201.9929          1270.1599          1538.9564
Red. masses --     1.3706             1.3461             1.1068
Frc consts  --     1.1667             1.2795             1.5444
IR Inten    --     2.5822            14.6708             7.9558
Raman Activ --     0.0000             0.0000             0.0000
Depolar     --     0.0000             0.0000             0.0000
```

```
Atom AN      X     Y     Z       X     Y     Z       X     Y     Z
  1  6    0.00  0.00  0.17    0.15  0.00  0.00    0.00  0.01  0.00
  2  1    0.00  0.00 -0.70   -0.25 -0.65  0.00    0.35  0.61  0.00
  3  1    0.00  0.00 -0.70   -0.25  0.65  0.00   -0.35  0.61  0.00
  4  8    0.00  0.00 -0.04   -0.08  0.00  0.00    0.00 -0.08  0.00
                     4                   5                   6
                    A'                  A'                  A'
Frequencies --  1826.6114           2870.0264           2919.5178
Red. masses --     7.4318              1.0428              1.1205
Frc consts  --    14.6096              5.0609              5.6271
IR Inten    --   110.4399             64.6212            169.5140
Raman Activ --     0.0000              0.0000              0.0000
Depolar     --     0.0000              0.0000              0.0000
Atom AN      X     Y     Z       X     Y     Z       X     Y     Z
  1  6    0.00  0.59  0.00    0.00  0.06  0.00    0.10  0.00  0.00
  2  1   -0.44 -0.22  0.00    0.61 -0.35  0.00   -0.60  0.37  0.00
  3  1    0.44 -0.22  0.00   -0.61 -0.35  0.00   -0.60 -0.37  0.00
  4  8    0.00 -0.42  0.00    0.00  0.00  0.00    0.00  0.00  0.00

-------------------
- Thermochemistry -
-------------------
Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
Atom  1 has atomic number  6 and mass  12.00000
Atom  2 has atomic number  1 and mass   1.00783
Atom  3 has atomic number  1 and mass   1.00783
Atom  4 has atomic number  8 and mass  15.99491
Molecular mass:    30.01056 amu.
Principal axes and moments of inertia in atomic units:
                      1       2       3
   EIGENVALUES --     6.34263  46.22062  52.56325
         X          0.00000   1.00000   0.00000
         Y          1.00000   0.00000   0.00000
         Z          0.00000   0.00000   1.00000
THIS MOLECULE IS AN ASYMMETRIC TOP.
ROTATIONAL SYMMETRY NUMBER  1.
ROTATIONAL TEMPERATURES (KELVIN)    13.65576    1.87391    1.64779
ROTATIONAL CONSTANTS (GHZ)         284.54142   39.04624   34.33466
Zero-point vibrational energy     69546.5 (Joules/Mol)
                                  16.62201 (Kcal/Mol)
VIBRATIONAL TEMPERATURES:   1729.39  1827.47  2214.20  2628.07  4129.30
       (KELVIN)          4200.51

Zero-point correction=                          0.026489 (Hartree/Particle)
Thermal correction to Energy=                   0.029356
Thermal correction to Enthalpy=                 0.030300
Thermal correction to Gibbs Free Energy=        0.004834
Sum of electronic and zero-point Energies=         -114.509853
Sum of electronic and thermal Energies=            -114.506985
Sum of electronic and thermal Enthalpies=          -114.506041
Sum of electronic and thermal Free Energies=       -114.531508

                 E (Thermal)             CV              S
                  KCAL/MOL        CAL/MOL-KELVIN    CAL/MOL-KELVIN
TOTAL                18.421            6.417           53.599
ELECTRONIC            0.000            0.000            0.000
TRANSLATIONAL         0.889            2.981           36.130
ROTATIONAL            0.889            2.981           17.384
VIBRATIONAL          16.644            0.456            0.085
                    Q          LOG10(Q)          LN(Q)
TOTAL BOT       0.598072D-02       -2.223246       -5.119214
TOTAL V=0       0.913486D+10        9.960702        22.935364
VIB (BOT)       0.658626D-12      -12.181361       -28.048620
VIB (V=0)       0.100597D+01        0.002587        0.005957
ELECTRONIC      0.100000D+01        0.000000        0.000000
TRANSLATIONAL   0.646207D+07        6.810372        15.681460
ROTATIONAL      0.140522D+04        3.147743        7.247946
***** Axes restored to original set *****
-------------------------------------------------------------------
Center     Atomic                 Forces (Hartrees/Bohr)
Number     Number              X           Y           Z
-------------------------------------------------------------------
  1        6         -0.000066222  -0.000167971   0.000000000
  2        1          0.000017528   0.000046124   0.000000000
```

```
  3        1        0.000014787   0.000041507   0.000000000
  4        8        0.000033908   0.000080340   0.000000000
---------------------------------------------------------------------
Cartesian Forces:  Max     0.000167971 RMS     0.000060951

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Internal  Forces:  Max     0.000087099 RMS     0.000043871
Search for a local minimum.
Step number   1 out of a maximum of  20
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Second derivative matrix not updated -- analytic derivatives used.
The second derivative matrix:
                R1       R2       R3       A1       A2
       R1        0.29778
       R2        0.00676   0.29777
       R3        0.03929   0.03929   0.88770
       A1        0.00866   0.00866  -0.03735   0.08611
       A2        0.00216  -0.01082   0.01868  -0.04306   0.11643
       A3       -0.01082   0.00216   0.01867  -0.04305  -0.07337
       A4        0.00000   0.00000   0.00000   0.00000   0.00000
                A3       A4
       A3        0.11643
       A4        0.00000   0.07027
   Eigenvalues ---    0.07027   0.12451   0.18816   0.29265   0.30140
   Eigenvalues ---    0.895491000.00000
Angle between quadratic step and forces=  37.17 degrees.
Linear search not attempted -- first point.
Iteration  1 RMS(Cart)=  0.00018939 RMS(Int)=  0.00000004
Iteration  2 RMS(Cart)=  0.00000004 RMS(Int)=  0.00000000
Variable      Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                       (Linear)    (Quad)   (Total)
  R1       2.09735   0.00003   0.00000   0.00012   0.00012   2.09747
  R2       2.09736   0.00002   0.00000   0.00012   0.00012   2.09747
  R3       2.26769  -0.00009   0.00000  -0.00014  -0.00014   2.26755
  A1       2.01604  -0.00006   0.00000  -0.00049  -0.00049   2.01555
  A2       2.13355   0.00003   0.00000   0.00027   0.00027   2.13382
  A3       2.13360   0.00002   0.00000   0.00022   0.00022   2.13382
  A4       3.14159   0.00000   0.00000   0.00000   0.00000   3.14159
      Item               Value     Threshold  Converged?
Maximum Force            0.000087     0.000450     YES
RMS     Force            0.000044     0.000300     YES
Maximum Displacement     0.000261     0.001800     YES
RMS     Displacement     0.000189     0.001200     YES
Predicted change in Energy=-2.940979D-08
Optimization completed.
   -- Stationary point found.
                 ----------------------------
                 !   Optimized Parameters   !
                 ! (Angstroms and Degrees)  !
-------------------------                        -------------------------
! Name  Definition           Value          Derivative Info.          !
-------------------------------------------------------------------------------
! R1    R(1,2)               1.1099         -DE/DX =    0.            !
! R2    R(1,3)               1.1099         -DE/DX =    0.            !
! R3    R(1,4)               1.2          -DE/DX =   -0.0001          !
! A1    A(2,1,3)           115.5104         -DE/DX =   -0.0001          !
! A2    A(2,1,4)           122.2433         -DE/DX =    0.            !
! A3    A(3,1,4)           122.2462         -DE/DX =    0.            !
! A4    L(3,1,4,2,-2)        180.           -DE/DX =    0.            !
-------------------------------------------------------------------------------
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

1|1|UNPC-UNK|Freq|RB3LYP|CBSB7|C1H2O1|PCUSER|11-Oct-2015|0||#N GEOM=AL
LCHECK GUESS=TCHECK B3LYP/CBSB7 FREQ||Title Card Required||0,1|C,0.180
6494346,0.4939903678,0.|H,-0.497601017,1.3725046282,0.|H,1.2656239041,
0.7277621471,0.|O,-0.2314899368,-0.6330261227,0.||Version=x86-Win32-G9
8RevA.11.4|State=1-A'|HF=-114.5363414|RMSD=2.220e-009|RMSF=6.095e-005|
Dipole=0.3026801,0.8276902,0.|DipoleDeriv=0.9136858,0.0503014,0.,0.050
2981,1.0328428,0.,0.,0.,0.1673203,-0.1298453,0.155473,0.,0.1321013,-0.
1601428,0.,0.,0.,0.074106,-0.2842001,-0.0507335,0.,-0.027369,-0.005785
5,0.,0.,0.,0.0741089,-0.4996404,-0.1550409,0.,-0.1550304,-0.8669145,0.
,0.,0.,-0.3155352|Polar=14.9978047,1.531609,18.6256175,0.,0.,7.9294655
|PG=CS [SG(C1H2O1)]||NImag=0||0.61903956,0.13585490,0.94085916,0.,0.,0.
```

17498267,-0.16649254,0.09952463,0.,0.15530026,0.10387192,-0.15978772,0
.,-0.11308703,0.20808743,0.,0.,-0.05856996,0.,0.,0.01959422,-0.2639541
1,-0.01158092,0.,-0.01616526,-0.00165803,0.,0.28874558,-0.01592979,-0.
06232332,0.,0.02051583,0.00617211,0.,0.04498809,0.07463467,0.,0.,-0.05
856910,0.,0.,0.01960487,0.,0.,0.01959520,-0.18859290,-0.22379861,0.,0.
02735754,0.01087315,0.,-0.00862621,-0.04957414,0.,0.16986157,-0.223797
03,-0.71874813,0.,-0.00695343,-0.05447182,0.,-0.03174914,-0.01848346,0
.,0.26249960,0.79170340,0.,0.,-0.05784361,0.,0.,0.01937088,0.,0.,0.019
36903,0.,0.,0.01910369||0.00006622,0.00016797,0.,-0.00001753,-0.000046
12,0.,-0.00001479,-0.00004151,0.,-0.00003391,-0.00008034,0.|||@

TO SEE A WORLD IN A GRAIN OF SAND
AND A HEAVEN IN A WILD FLOWER
HOLD INFINITY IN THE PALM OF YOUR HAND
AND ETERNITY IN AN HOUR

-- WILLIAM BLAKE

Job cpu time: 0 days 0 hours 0 minutes 17.0 seconds.
File lengths (MBytes): RWF= 6 Int= 0 D2E= 0 Chk= 3 Scr= 1
Normal termination of Gaussian 98.
Link1: Proceeding to internal job step number 3.

#N Geom=AllCheck Guess=TCheck CCSD(T)/6-31+G(d')

1/29=7,38=1/1;
2/40=1/2;
3/5=11,6=6,7=11,11=9,25=1,30=1/1,2,3;
4/5=101/1;
5/5=2/2;
8/6=7,9=120000,10=1,27=262144000/1,4;
9/5=7,14=2,27=262144000/13;
6/7=2,8=2,9=2,10=2/1;
99/5=1,9=1/99;

Title Card Required

Redundant internal coordinates taken from checkpoint file:
C:\Users\hp\Desktop\1_cbsqb3.chk
Charge = 0 Multiplicity = 1
C,0,0.1806494346,0.4939903678,0.
H,0,-0.497601017,1.3725046282,0.
H,0,1.2656239041,0.7277621471,0.
O,0,-0.2314899368,-0.6330261227,0.
Recover connectivity data from disk.

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.180649	0.493990	0.000000
2	1	0	-0.497601	1.372505	0.000000
3	1	0	1.265624	0.727762	0.000000
4	8	0	-0.231490	-0.633026	0.000000

Distance matrix (angstroms):

	1	2	3	4
1 C	0.000000			
2 H	1.109870	0.000000		
3 H	1.109873	1.877406	0.000000	
4 O	1.200010	2.023109	2.023140	0.000000

Interatomic angles:
H2-C1-H3=115.5104 H2-C1-O4=122.2433 H3-C1-O4=122.2462
H3-H2-O4= 62.3562
Stoichiometry CH2O
Framework group CS[SG(CH2O)]
Deg. of freedom 5
Full point group CS NOp 2
Largest Abelian subgroup CS NOp 2
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

```
---------------------------------------------------------------------
  1       6          0      0.000002    0.525985    0.000000
  2       1          0     -0.938715    1.118119    0.000000
  3       1          0      0.938691    1.118168    0.000000
  4       8          0      0.000002   -0.674025    0.000000
---------------------------------------------------------------------
Rotational constants (GHZ):    284.5414197     39.0462381     34.3346594
Isotopes: C-12,H-1,H-1,O-16
Standard basis: 6-31+(d') (6D, 7F)
There are    32 symmetry adapted basis functions of A'  symmetry.
There are    10 symmetry adapted basis functions of A"  symmetry.
Crude estimate of integral set expansion from redundant integrals=1.000.
Integral buffers will be    262144 words long.
Raffenetti 1 integral format.
Two-electron integral symmetry is turned on.
   42 basis functions       72 primitive gaussians
    8 alpha electrons       8 beta electrons
      nuclear repulsion energy       31.3552993902 Hartrees.
One-electron integrals computed using PRISM.
NBasis=    42 RedAO= T  NBF=    32    10
NBsUse=    42 1.00D-04 NBFU=    32    10
Initial guess read from the checkpoint file:
C:\Users\hp\Desktop\1_cbsqb3.chk
Unable to project full set of read-in orbitals.
Projecting just the   8 occupied ones.
Initial guess orbital symmetries:
     Occupied  (A') (A') (A') (A') (A') (A') (A") (A')
     Virtual   (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A") (A") (A") (A") (A")
               (A") (A") (A") (A")
Requested convergence on RMS density matrix=1.00D-08 within  64 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Keep R1 integrals in memory in canonical form, NReq=      848588.
SCF Done:  E(RHF) =  -113.871164641     A.U. after   11 cycles
         Convg  =    0.3485D-08           -V/T =  2.0028
         S**2   =   0.0000
Range of M.O.s used for correlation:    3    42
NBasis=    42 NAE=     8 NBE=     8 NFC=     2 NFV=     0
NROrb=     40 NOA=     6 NOB=     6 NVA=    34 NVB=    34
Estimate disk for full transformation     2934594 words.
Spin components of T(2) and E(2):
   alpha-alpha T2 =       0.1209445813D-01 E2=     -0.3992722271D-01
   alpha-beta  T2 =       0.7292303350D-01 E2=     -0.2342800200D+00
   beta-beta   T2 =       0.1209445813D-01 E2=     -0.3992722271D-01
ANorm=    0.1047431119D+01
E2=      -0.3141344654D+00 EUMP2=      -0.11418529910605D+03
Iterations=  50 Convergence= 0.100D-06
Iteration Nr.   1
**********************
MP4(R+Q)=  0.46523836D-02
E3=      -0.46000451D-02       EUMP3=     -0.11418989915D+03
E4(DQ)=   -0.41219943D-02       UMP4(DQ)=   -0.11419402115D+03
E4(SDQ)=  -0.90397875D-02       UMP4(SDQ)=  -0.11419893894D+03
DE(CORR)= -0.31372624D+00       E(CORR)=    -0.11418489088D+03
NORM(A)=   0.10497682D+01
Iteration Nr.   2
**********************
DE(CORR)= -0.32493786D+00       E(CORR)=    -0.11419610250D+03
NORM(A)=   0.10556990D+01
Iteration Nr.   3
**********************
DE(CORR)= -0.32578513D+00       E(CORR)=    -0.11419694977D+03
NORM(A)=   0.10575533D+01
Iteration Nr.   4
**********************
DE(CORR)= -0.32695846D+00       E(CORR)=    -0.11419812310D+03
NORM(A)=   0.10580829D+01
Iteration Nr.   5
**********************
DE(CORR)= -0.32709058D+00       E(CORR)=    -0.11419825522D+03
NORM(A)=   0.10582300D+01
Iteration Nr.   6
**********************
```

```
DE(CORR)= -0.32710549D+00      E(CORR)=    -0.11419827013D+03
NORM(A)=   0.10582371D+01
Iteration Nr.   7
**********************
DE(CORR)= -0.32710572D+00      E(CORR)=    -0.11419827036D+03
NORM(A)=   0.10582390D+01
Iteration Nr.   8
**********************
DE(CORR)= -0.32710394D+00      E(CORR)=    -0.11419826858D+03
NORM(A)=   0.10582407D+01
Iteration Nr.   9
**********************
DE(CORR)= -0.32710448D+00      E(CORR)=    -0.11419826912D+03
NORM(A)=   0.10582413D+01
Iteration Nr.  10
**********************
DE(CORR)= -0.32710452D+00      E(CORR)=    -0.11419826917D+03
NORM(A)=   0.10582416D+01
Iteration Nr.  11
**********************
DE(CORR)= -0.32710476D+00      E(CORR)=    -0.11419826940D+03
NORM(A)=   0.10582418D+01
Iteration Nr.  12
**********************
DE(CORR)= -0.32710480D+00      E(CORR)=    -0.11419826944D+03
NORM(A)=   0.10582419D+01
Largest amplitude= 6.65D-02
Time for triples=       1.00 seconds.
T4(CCSD)= -0.11452138D-01
T5(CCSD)=  0.11205481D-02
CCSD(T)= -0.11420860103D+03

**********************************************************************

        Population analysis using the SCF density.

**********************************************************************

Orbital Symmetries:
    Occupied  (A') (A') (A') (A') (A') (A') (A") (A')
    Virtual   (A") (A') (A') (A') (A") (A') (A') (A') (A") (A')
           (A') (A') (A") (A') (A') (A') (A') (A') (A') (A")
           (A') (A") (A") (A') (A') (A') (A') (A") (A') (A')
           (A") (A') (A') (A')
 The electronic state is 1-A'.
Alpha  occ. eigenvalues --  -20.59105 -11.35100  -1.41672  -0.87096  -0.69616
Alpha  occ. eigenvalues --   -0.65692  -0.54170  -0.44305
Alpha virt. eigenvalues --    0.07398   0.07778   0.09983   0.10379   0.16849
Alpha virt. eigenvalues --    0.28311   0.30685   0.31996   0.32929   0.38901
Alpha virt. eigenvalues --    0.39281   0.52616   0.85730   0.93051   0.94428
Alpha virt. eigenvalues --    1.13278   1.13608   1.23755   1.42488   1.46561
Alpha virt. eigenvalues --    1.48652   1.49343   1.62903   1.85247   1.97983
Alpha virt. eigenvalues --    2.20734   2.41896   3.21530   3.24225   3.51199
Alpha virt. eigenvalues --    3.63685   3.71390   4.10878   6.65456
       Condensed to atoms (all electrons):
             1        2        3        4
 1  C    4.918791   0.386569   0.386564   0.405896
 2  H    0.386569   0.547180  -0.061118  -0.056084
 3  H    0.386564  -0.061118   0.547178  -0.056080
 4  O    0.405896  -0.056084  -0.056080   7.975355
Total atomic charges:
             1
 1  C   -0.097820
 2  H    0.183452
 3  H    0.183455
 4  O   -0.269087
Sum of Mulliken charges=   0.00000
Atomic charges with hydrogens summed into heavy atoms:
             1
 1  C    0.269087
 2  H    0.000000
 3  H    0.000000
 4  O   -0.269087
Sum of Mulliken charges=   0.00000
```

Electronic spatial extent (au): <R**2>= 60.6161
Charge= 0.0000 electrons
Dipole moment (Debye):
X= 0.0000 Y= 2.9333 Z= 0.0000 Tot= 2.9333
Quadrupole moment (Debye-Ang):
XX= -11.5814 YY= -12.2443 ZZ= -11.7999
XY= 0.0001 XZ= 0.0000 YZ= 0.0000
Octapole moment (Debye-Ang**2):
XXX= 0.0000 YYY= 0.3889 ZZZ= 0.0000 XYY= 0.0001
XXY= 0.7960 XXZ= 0.0000 XZZ= 0.0000 YZZ= -0.4384
YYZ= 0.0000 XYZ= 0.0000
Hexadecapole moment (Debye-Ang**3):
XXXX= -17.7631 YYYY= -45.2365 ZZZZ= -10.5119 XXXY= 0.0000
XXXZ= 0.0000 YYYX= 0.0002 YYYZ= 0.0000 ZZZX= 0.0000
ZZZY= 0.0000 XXYY= -10.0760 XXZZ= -5.0284 YYZZ= -9.3586
XXYZ= 0.0000 YYXZ= 0.0000 ZZXY= 0.0000
N-N= 3.135529939020D+01 E-N=-3.308725743720D+02 KE= 1.135547747706D+02
Symmetry A' KE= 1.100675569426D+02
Symmetry A" KE= 3.487217828036D+00
1|1|UNPC-UNK|SP|RCCSD(T)-FC|6-31+(d')|C1H2O1|PCUSER|11-Oct-2015|0||#N
GEOM=ALLCHECK GUESS=TCHECK CCSD(T)/6-31+G(D')||Title Card Required||0,
1|C,0.1806494346,0.4939903678,0.|H,-0.497601017,1.3725046282,0.|H,1.26
56239041,0.7277621471,0.|O,-0.2314899368,-0.6330261227,0.||Version=x86
-Win32-G98RevA.11.4|State=1-A'|HF=-113.8711646|MP2=-114.1852991|MP3=-1
14.1898992|MP4D=-114.1986735|MP4DQ=-114.1940211|MP4SDQ=-114.1989389|CC
SD=-114.1982694|CCSD(T)=-114.208601|RMSD=3.485e-009|PG=CS [SG(C1H2O1)]
||@

TO SEE A WORLD IN A GRAIN OF SAND
AND A HEAVEN IN A WILD FLOWER
HOLD INFINITY IN THE PALM OF YOUR HAND
AND ETERNITY IN AN HOUR

-- WILLIAM BLAKE
Job cpu time: 0 days 0 hours 0 minutes 4.0 seconds.
File lengths (MBytes): RWF= 19 Int= 0 D2E= 0 Chk= 3 Scr= 1
Normal termination of Gaussian 98.
Link1: Proceeding to internal job step number 4.

#N Geom=AllCheck Guess=TCheck MP4SDQ/CBSB4

1/29=7,38=1/1;
2/40=1/2;
3/5=13,11=9,25=1,30=1/1,2,3;
4/5=101/1;
5/5=2/2;
8/6=3,9=120000,10=1,27=262144000/1,4;
9/5=4,27=262144000/13;
6/7=2,8=2,9=2,10=2/1;
99/5=1,9=1/99;

Title Card Required

Redundant internal coordinates taken from checkpoint file:
C:\Users\hp\Desktop\1_cbsqb3.chk
Charge = 0 Multiplicity = 1
C,0,0.1806494346,0.4939903678,0.
H,0,-0.497601017,1.3725046282,0.
H,0,1.2656239041,0.7277621471,0.
O,0,-0.2314899368,-0.6330261227,0.
Recover connectivity data from disk.
Input orientation:

Center Atomic Atomic Coordinates (Angstroms)
Number Number Type X Y Z
---
1 6 0 0.180649 0.493990 0.000000
2 1 0 -0.497601 1.372505 0.000000
3 1 0 1.265624 0.727762 0.000000
4 8 0 -0.231490 -0.633026 0.000000

Distance matrix (angstroms):
1 2 3 4

```
  1  C   0.000000
  2  H   1.109870  0.000000
  3  H   1.109873  1.877406  0.000000
  4  O   1.200010  2.023109  2.023140  0.000000
                Interatomic angles:
   H2-C1-H3=115.5104      H2-C1-O4=122.2433      H3-C1-O4=122.2462
   H3-H2-O4= 62.3562
Stoichiometry    CH2O
Framework group  CS[SG(CH2O)]
Deg. of freedom   5
Full point group              CS     NOp   2
Largest Abelian subgroup      CS     NOp   2
Largest concise Abelian subgroup C1     NOp   1
                Standard orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic          Coordinates (Angstroms)
Number     Number     Type            X         Y         Z
---------------------------------------------------------------------
  1        6          0       0.000002    0.525985    0.000000
  2        1          0      -0.938715    1.118119    0.000000
  3        1          0       0.938691    1.118168    0.000000
  4        8          0       0.000002   -0.674025    0.000000
---------------------------------------------------------------------
Rotational constants (GHZ):    284.5414197     39.0462381     34.3346594
Isotopes: C-12,H-1,H-1,O-16
Standard basis: CBSB4 (6D, 7F)
There are    36 symmetry adapted basis functions of A'  symmetry.
There are    12 symmetry adapted basis functions of A"  symmetry.
Crude estimate of integral set expansion from redundant integrals=1.000.
Integral buffers will be    262144 words long.
Raffenetti 1 integral format.
Two-electron integral symmetry is turned on.
   48 basis functions       78 primitive gaussians
    8 alpha electrons       8 beta electrons
     nuclear repulsion energy       31.3552993902 Hartrees.
One-electron integrals computed using PRISM.
NBasis=    48 RedAO= T  NBF=    36    12
NBsUse=    48 1.00D-04 NBFU=    36    12
Initial guess read from the checkpoint file:
C:\Users\hp\Desktop\1_cbsqb3.chk
Initial guess orbital symmetries:
     Occupied  (A') (A') (A') (A') (A') (A') (A") (A')
     Virtual   (A") (A') (A') (A') (A") (A') (A') (A') (A") (A')
           (A') (A') (A") (A') (A') (A') (A') (A') (A') (A")
           (A') (A") (A") (A') (A') (A') (A') (A") (A') (A')
           (A") (A') (A') (A') (A') (A') (A') (A') (A") (A")
Requested convergence on RMS density matrix=1.00D-08 within  64 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Keep R1 integrals in memory in canonical form, NReq=     1134318.
SCF Done:  E(RHF) =  -113.874206449     A.U. after    9 cycles
         Convg  =    0.8369D-08           -V/T =  2.0028
         S**2   =   0.0000
Range of M.O.s used for correlation:    3    48
NBasis=    48 NAE=     8 NBE=     8 NFC=     2 NFV=     0
NROrb=     46 NOA=     6 NOB=     6 NVA=    40 NVB=    40
Spin components of T(2) and E(2):
   alpha-alpha T2 =       0.1226591545D-01 E2=     -0.4053279363D-01
   alpha-beta  T2 =       0.7566565709D-01 E2=     -0.2456486194D+00
   beta-beta   T2 =       0.1226591545D-01 E2=     -0.4053279363D-01
ANorm=    0.1048902993D+01
E2=      -0.3267142067D+00 EUMP2=      -0.11420092065611D+03
R2 and R3 integrals will be kept in memory, NReq=     1814152.
DD1Dir will call FoFMem   1 times, MxPair=       42
NAB=    21 NAA=     0 NBB=     0.
MP4(R+Q)=  0.51508087D-02
E3=      -0.60530403D-02       EUMP3=      -0.11420697370D+03
E4(DQ)=   -0.38707442D-02       UMP4(DQ)=   -0.11421084444D+03
E4(SDQ)=  -0.88410643D-02       UMP4(SDQ)=  -0.11421581476D+03
Largest amplitude= 5.10D-02

**********************************************************************

        Population analysis using the SCF density.
```

```
**********************************************************************

Orbital Symmetries:
    Occupied  (A') (A') (A') (A') (A') (A') (A") (A')
    Virtual   (A") (A') (A') (A') (A") (A') (A') (A') (A") (A')
          (A') (A') (A") (A') (A') (A') (A') (A') (A") (A')
          (A") (A') (A") (A') (A') (A') (A") (A') (A") (A')
          (A') (A') (A') (A") (A') (A") (A') (A') (A') (A')
 The electronic state is 1-A'.
Alpha  occ. eigenvalues --  -20.59097 -11.35109  -1.41656  -0.87063  -0.69543
Alpha  occ. eigenvalues --   -0.65642  -0.54143  -0.44243
Alpha virt. eigenvalues --    0.07344   0.07729   0.09980   0.10311   0.16834
Alpha virt. eigenvalues --    0.28293   0.30632   0.31978   0.32912   0.38810
Alpha virt. eigenvalues --    0.39211   0.52603   0.85728   0.92474   0.92679
Alpha virt. eigenvalues --    1.07071   1.07151   1.23342   1.23852   1.41710
Alpha virt. eigenvalues --    1.47706   1.48576   1.52682   1.74499   1.80714
Alpha virt. eigenvalues --    1.84549   2.02568   2.10155   2.10603   2.11310
Alpha virt. eigenvalues --    2.68300   2.83563   2.84668   3.24778   3.30638
Alpha virt. eigenvalues --    3.64993   3.69275   3.94450   4.11879   6.69773
        Condensed to atoms (all electrons):
             1        2        3        4
 1  C    4.668671   0.412281   0.412277   0.406472
 2  H    0.412281   0.616656  -0.064138  -0.058748
 3  H    0.412277  -0.064138   0.616653  -0.058742
 4  O    0.406472  -0.058748  -0.058742   7.999214
Total atomic charges:
             1
 1  C    0.100299
 2  H    0.093948
 3  H    0.093949
 4  O   -0.288196
Sum of Mulliken charges=   0.00000
Atomic charges with hydrogens summed into heavy atoms:
             1
 1  C    0.288196
 2  H    0.000000
 3  H    0.000000
 4  O   -0.288196
Sum of Mulliken charges=   0.00000
Electronic spatial extent (au):  <R**2>=    60.5986
Charge=     0.0000 electrons
Dipole moment (Debye):
   X=     0.0000    Y=     2.9303    Z=     0.0000  Tot=     2.9303
Quadrupole moment (Debye-Ang):
  XX=   -11.5597   YY=   -12.2667   ZZ=   -11.7756
  XY=     0.0001   XZ=     0.0000   YZ=     0.0000
Octapole moment (Debye-Ang**2):
 XXX=    -0.0001  YYY=     0.3495  ZZZ=     0.0000  XYY=     0.0001
 XXY=     0.8225  XXZ=     0.0000  XZZ=     0.0000  YZZ=    -0.4296
 YYZ=     0.0000  XYZ=     0.0000
Hexadecapole moment (Debye-Ang**3):
XXXX=   -17.8092 YYYY=   -45.4418 ZZZZ=   -10.4414 XXXY=     0.0000
XXXZ=     0.0000 YYYX=     0.0002 YYYZ=     0.0000 ZZZX=     0.0000
ZZZY=     0.0000 XXYY=   -10.0700 XXZZ=    -5.0522 YYZZ=    -9.3751
XXYZ=     0.0000 YYXZ=     0.0000 ZZXY=     0.0000
N-N= 3.135529939020D+01 E-N=-3.308908598503D+02  KE= 1.135617823511D+02
Symmetry A'   KE= 1.100771601808D+02
Symmetry A"   KE= 3.484622170328D+00
1|1|UNPC-UNK|SP|RMP4SDQ-FC|CBSB4|C1H2O1|PCUSER|11-Oct-2015|0||#N GEOM=
ALLCHECK GUESS=TCHECK MP4SDQ/CBSB4||Title Card Required||0,1|C,0.18064
94346,0.4939903678,0.|H,-0.497601017,1.3725046282,0.|H,1.2656239041,0.
7277621471,0.|O,-0.2314899368,-0.6330261227,0.||Version=x86-Win32-G98R
evA.11.4|State=1-A'|HF=-113.8742064|MP2=-114.2009207|MP3=-114.2069737|
MP4D=-114.2159952|MP4DQ=-114.2108444|MP4SDQ=-114.2158148|RMSD=8.369e-0
09|PG=CS [SG(C1H2O1)]||@


TO SEE A WORLD IN A GRAIN OF SAND
AND A HEAVEN IN A WILD FLOWER
HOLD INFINITY IN THE PALM OF YOUR HAND
AND ETERNITY IN AN HOUR

                -- WILLIAM BLAKE
Job cpu time:  0 days  0 hours  0 minutes  1.0 seconds.
```

File lengths (MBytes): RWF=   19 Int=   0 D2E=   0 Chk=   3 Scr=   1
Normal termination of Gaussian 98.
Link1: Proceeding to internal job step number 5.

#N Geom=AllCheck Guess=TCheck MP2/CBSB3 CBSExtrap=(NMin=10,MinPop)

1/29=7,38=1/1;
2/40=1/2;
3/5=12,11=9,25=1,30=1/1,2,3;
4/5=101/1;
5/5=2/2;
8/10=1,27=262144000,41=10,43=4/1,4,3;
6/7=2,8=2,9=2,10=2/1;
99/5=1,9=1/99;

Title Card Required

Redundant internal coordinates taken from checkpoint file:
C:\Users\hp\Desktop\1_cbsqb3.chk
Charge = 0 Multiplicity = 1
C,0,0.1806494346,0.4939903678,0.
H,0,-0.497601017,1.3725046282,0.
H,0,1.2656239041,0.7277621471,0.
O,0,-0.2314899368,-0.6330261227,0.
Recover connectivity data from disk.
                    Input orientation:

Center   Atomic   Atomic   Coordinates (Angstroms)
Number   Number   Type   X   Y   Z
---
  1   6   0   0.180649   0.493990   0.000000
  2   1   0   -0.497601   1.372505   0.000000
  3   1   0   1.265624   0.727762   0.000000
  4   8   0   -0.231490   -0.633026   0.000000

             Distance matrix (angstroms):
                  1   2   3   4
   1 C   0.000000
   2 H   1.109870   0.000000
   3 H   1.109873   1.877406   0.000000
   4 O   1.200010   2.023109   2.023140   0.000000
                    Interatomic angles:
    H2-C1-H3=115.5104   H2-C1-O4=122.2433   H3-C1-O4=122.2462
    H3-H2-O4= 62.3562
Stoichiometry   CH2O
Framework group CS[SG(CH2O)]
Deg. of freedom   5
Full point group   CS   NOp   2
Largest Abelian subgroup   CS   NOp   2
Largest concise Abelian subgroup C1   NOp   1
                   Standard orientation:

Center   Atomic   Atomic   Coordinates (Angstroms)
Number   Number   Type   X   Y   Z
---
  1   6   0   0.000002   0.525985   0.000000
  2   1   0   -0.938715   1.118119   0.000000
  3   1   0   0.938691   1.118168   0.000000
  4   8   0   0.000002   -0.674025   0.000000

Rotational constants (GHZ):   284.5414197   39.0462381   34.3346594
Isotopes: C-12,H-1,H-1,O-16
Standard basis: CBSB3 (5D, 7F)
There are   62 symmetry adapted basis functions of A' symmetry.
There are   26 symmetry adapted basis functions of A" symmetry.
Crude estimate of integral set expansion from redundant integrals=1.000.
Integral buffers will be   262144 words long.
Raffenetti 1 integral format.
Two-electron integral symmetry is turned on.
   88 basis functions   128 primitive gaussians
    8 alpha electrons   8 beta electrons
     nuclear repulsion energy   31.3552993902 Hartrees.
One-electron integrals computed using PRISM.
NBasis=   88 RedAO= T NBF=   62   26

```
NBsUse=   88 1.00D-04 NBFU=   62   26
Initial guess read from the checkpoint file:
C:\Users\hp\Desktop\1_cbsqb3.chk
Initial guess orbital symmetries:
     Occupied  (A') (A') (A') (A') (A') (A') (A") (A')
     Virtual   (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A") (A") (A") (A") (A")
               (A") (A") (A") (A") (A") (A") (A") (A") (A") (A")
               (A") (A") (A") (A") (A") (A") (A") (A") (A") (A")
Requested convergence on RMS density matrix=1.00D-08 within  64 cycles.
Requested convergence on MAX density matrix=1.00D-06.
SCF Done:  E(RHF) =  -113.909678285     A.U. after    9 cycles
          Convg  =    0.9411D-08           -V/T =  2.0015
          S**2   =   0.0000
Range of M.O.s used for correlation:    3   88
NBasis=   88 NAE=    8 NBE=    8 NFC=    2 NFV=    0
NROrb=    86 NOA=    6 NOB=    6 NVA=   80 NVB=   80

**** Warning!!: The largest alpha MO coefficient is  0.11282403D+02

Semi-Direct transformation.
ModeAB=          2 MOrb=           6 LenV=      5988149
LASXX=      285120 LTotXX=     285120 LenRXX=     285120
LTotAB=     308961 MaxLAS=    2503116 LenRXY=    2503116
NonZer=    2611476 LenScr=    4894720 LnRSAI=         0
LnScr1=         0 LExtra=     727425 Total=     8410381
MaxDsk=   262144000 SrtSym=          F ITran=          3
JobTyp=0 Pass  1:  I=   1 to   6.
(rs|ai) integrals will be sorted in core.
Spin components of T(2) and E(2):
   alpha-alpha T2 =       0.1348662200D-01 E2=     -0.4712661709D-01
   alpha-beta  T2 =       0.8301817327D-01 E2=     -0.2960877515D+00
   beta-beta   T2 =       0.1348662200D-01 E2=     -0.4712661709D-01
ANorm=    0.1053561302D+01
E2=      -0.3903409857D+00 EUMP2=      -0.11430001927106D+03

Complete Basis Set (CBS) Extrapolation:
M. R. Nyden and G. A. Petersson, JCP 75, 1843 (1981)
G. A. Petersson and M. A. Al-Laham, JCP 94, 6081 (1991)
G. A. Petersson, T. Tensfeldt, and J. A. Montgomery, JCP 94, 6091 (1991)
J. A. Montgomery, J. W. Ochterski, and G. A. Petersson, JCP 101, 5900 (1994)

Minimum Number of PNO for Extrapolation =  10
Absolute Overlaps: IRadAn =     99302
LocTrn: ILocal=3 LocCor=F DoCore=F.
LocMO: Using population method
Initial Trace= 0.60000000D+01 Initial TraceA= 0.28338124D+01
RMSG= 0.71044963D-08
E2(CBS)=     -0.429440 CBS-Int=      0.012639 OIii=      3.337527

******************************************************************************

        Population analysis using the SCF density.

******************************************************************************

Orbital Symmetries:
     Occupied  (A') (A') (A') (A') (A') (A') (A") (A')
     Virtual   (A') (A') (A") (A') (A') (A") (A') (A') (A') (A')
               (A") (A') (A') (A') (A') (A') (A") (A") (A') (A')
               (A") (A') (A') (A') (A') (A") (A") (A') (A') (A")
               (A') (A') (A') (A') (A') (A") (A') (A") (A') (A')
               (A') (A') (A") (A") (A") (A') (A') (A') (A') (A")
               (A") (A') (A') (A") (A') (A') (A') (A") (A") (A')
               (A') (A') (A') (A") (A") (A') (A') (A') (A") (A')
               (A") (A') (A") (A') (A') (A") (A') (A') (A') (A')
 The electronic state is 1-A'.
Alpha  occ. eigenvalues --  -20.57894 -11.34279  -1.41158  -0.86872  -0.69417
Alpha  occ. eigenvalues --   -0.65528  -0.54112  -0.44266
Alpha virt. eigenvalues --    0.04058   0.06464   0.07421   0.09855   0.15891
```

Alpha virt. eigenvalues -- 0.15996 0.16285 0.23840 0.27590 0.29557
Alpha virt. eigenvalues -- 0.32079 0.38104 0.38139 0.49267 0.61191
Alpha virt. eigenvalues -- 0.62334 0.69136 0.69545 0.72658 0.74383
Alpha virt. eigenvalues -- 0.93747 0.94547 1.02850 1.05451 1.15311
Alpha virt. eigenvalues -- 1.16698 1.17583 1.26948 1.28383 1.33575
Alpha virt. eigenvalues -- 1.44597 1.58616 1.63362 1.65791 1.81959
Alpha virt. eigenvalues -- 1.95182 2.09444 2.21591 2.46730 2.71472
Alpha virt. eigenvalues -- 2.74015 2.81169 3.03009 3.18016 3.19753
Alpha virt. eigenvalues -- 3.31790 3.33438 3.36923 3.42238 3.51623
Alpha virt. eigenvalues -- 3.58359 3.58544 3.85280 3.88570 4.05086
Alpha virt. eigenvalues -- 4.13195 4.35692 4.40324 4.44403 4.51126
Alpha virt. eigenvalues -- 4.88133 5.30125 5.47444 5.50048 5.58064
Alpha virt. eigenvalues -- 5.69493 5.85119 5.86474 5.88222 6.31319
Alpha virt. eigenvalues -- 6.73169 7.02487 7.34823 7.38017 7.49725
Alpha virt. eigenvalues -- 7.69546 7.87615 8.12267 25.64364 51.81399
Condensed to atoms (all electrons):

		1	2	3	4
1	C	4.547431	0.417230	0.417225	0.430871
2	H	0.417230	0.663431	-0.087983	-0.057426
3	H	0.417225	-0.087983	0.663427	-0.057419
4	O	0.430871	-0.057426	-0.057419	8.000713

Total atomic charges:

		1
1	C	0.187243
2	H	0.064748
3	H	0.064749
4	O	-0.316740

Sum of Mulliken charges= 0.00000
Atomic charges with hydrogens summed into heavy atoms:

		1
1	C	0.316740
2	H	0.000000
3	H	0.000000
4	O	-0.316740

Sum of Mulliken charges= 0.00000
Electronic spatial extent (au): <R**2>= 60.4066
Charge= 0.0000 electrons
Dipole moment (Debye):
X= 0.0000 Y= 2.8542 Z= 0.0000 Tot= 2.8542
Quadrupole moment (Debye-Ang):
XX= -11.4810 YY= -12.1077 ZZ= -11.7551
XY= 0.0001 XZ= 0.0000 YZ= 0.0000
Octapole moment (Debye-Ang**2):
XXX= -0.0001 YYY= 0.1063 ZZZ= 0.0000 XYY= 0.0001
XXY= 0.8512 XXZ= 0.0000 XZZ= 0.0000 YZZ= -0.4264
YYZ= 0.0000 XYZ= 0.0000
Hexadecapole moment (Debye-Ang**3):
XXXX= -17.6557 YYYY= -45.1002 ZZZZ= -10.4666 XXXY= 0.0000
XXXZ= 0.0000 YYYX= 0.0002 YYYZ= 0.0000 ZZZX= 0.0000
ZZZY= 0.0000 XXYY= -9.9139 XXZZ= -5.0834 YYZZ= -9.2772
XXYZ= 0.0000 YYXZ= 0.0000 ZZXY= 0.0000
N-N= 3.135529939020D+01 E-N=-3.311957237345D+02 KE= 1.137362787549D+02
Symmetry A' KE= 1.102423031980D+02
Symmetry A" KE= 3.493975556911D+00
1|1|UNPC-UNK|SP|RMP2-FC|CBSB3|C1H2O1|PCUSER|11-Oct-2015|0||#N GEOM=ALL
CHECK GUESS=TCHECK MP2/CBSB3 CBSEXTRAP=(NMIN=10,MINPOP)||Title Card Re
quired||0,1|C,0.1806494346,0.4939903678,0.|H,-0.497601017,1.3725046282
,0.|H,1.2656239041,0.7277621471,0.|O,-0.2314899368,-0.6330261227,0.||V
ersion=x86-Win32-G98RevA.11.4|State=1-A'|HF=-113.9096783|MP2=-114.3000
193|E2(CBS)=-0.4294401|CBS-Int=-0.4168009|Oiii=3.3375268|RMSD=9.411e-0
09|PG=CS [SG(C1H2O1)]||@

MAN IS A SINGULAR CREATURE. HE HAS A SET OF GIFTS
WHICH MAKE HIM UNIQUE AMONG THE ANIMALS: SO THAT,
UNLIKE THEM, HE IS NOT A FIGURE IN THE LANDSCAPE --
HE IS A SHAPER OF THE LANDSCAPE.

-- JACOB BRONOWSKI

Complete Basis Set (CBS) Extrapolation:
M. R. Nyden and G. A. Petersson, JCP 75, 1843 (1981)
G. A. Petersson and M. A. Al-Laham, JCP 94, 6081 (1991)
G. A. Petersson, T. Tensfeldt, and J. A. Montgomery, JCP 94, 6091 (1991)

J. A. Montgomery, J. W. Ochterski, and G. A. Petersson, JCP 101, 5900 (1994)

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.026224 E(Thermal)= 0.029093
E(SCF)= -113.909678 DE(MP2)= -0.390341
DE(CBS)= -0.039099 DE(MP34)= -0.014894
DE(CCSD)= -0.009662 DE(Int)= 0.012639
DE(Empirical)= -0.019324
CBS-QB3 (0 K)= -114.344136 CBS-QB3 Energy= -114.341267
CBS-QB3 Enthalpy= -114.340322 CBS-QB3 Free Energy= -114.365791
1|1|UNPC-UNK|Mixed|CBS-QB3|CBS-QB3|C1H2O1|PCUSER|11-Oct-2015|0||# OPT
FREQ CBS-QB3 GEOM=CONNECTIVITY||Title Card Required||0,1|C,0.180649434
6,0.4939903678,0.|H,-0.497601017,1.3725046282,0.|H,1.2656239041,0.7277
621471,0.|O,-0.2314899368,-0.6330261227,0.||Version=x86-Win32-G98RevA.
11.4|State=1-A'|HF/CbsB3=-113.9096783|E2(CBS)/CbsB3=-0.4294401|CBS-Int
/CbsB3=0.0126393|OIii/CbsB3=3.3375268|MP2/CbsB4=-114.2009207|MP4(SDQ)/
CbsB4=-114.2158148|MP4(SDQ)/6-31+G(d')=-114.1989389|QCISD(T)/6-31+G(d'
)=-114.208601|CBSQB3=-114.3441356|FreqCoord=0.3413779313,0.9335064361,
0.,-0.9403295738,2.5936576654,0.,2.3916823833,1.3752710429,0.,-0.43745
25497,-1.1962459156,0.|PG=CS [SG(C1H2O1)]|NImag=0||0.61903956,0.135854
90,0.94085916,0.,0.,0.17498267,-0.16649254,0.09952463,0.,0.15530026,0.
10387192,-0.15978772,0.,-0.11308703,0.20808743,0.,0.,-0.05856996,0.,0.
,0.01959422,-0.26395411,-0.01158092,0.,-0.01616526,-0.00165803,0.,0.28
874558,-0.01592979,-0.06232332,0.,0.02051583,0.00617211,0.,0.04498809,
0.07463467,0.,0.,-0.05856910,0.,0.,0.01960487,0.,0.,0.01959520,-0.1885
9290,-0.22379861,0.,0.02735754,0.01087315,0.,-0.00862621,-0.04957414,0
.,0.16986157,-0.22379703,-0.71874813,0.,-0.00695343,-0.05447182,0.,-0.
03174914,-0.01848346,0.,0.26249960,0.79170340,0.,0.,-0.05784361,0.,0.,
0.01937088,0.,0.,0.01936903,0.,0.,0.01910369||0.00006622,0.00016797,0.
,-0.00001753,-0.00004612,0.,-0.00001479,-0.00004151,0.,-0.00003391,-0.
00008034,0.|||@
Job cpu time: * days * hours * minutes * seconds.
File lengths (MBytes): RWF= 67 Int= 0 D2E= 0 Chk= 3 Scr= 1
Normal termination of Gaussian 98.

Electronic Supporting Information

Appendix II

OUT PUT file of Formaldehyde Trimer by the CBS-QB3 method

Entering Link 1 = C:\G98W\l1.exe PID= 6140.

Copyright (c) 1988,1990,1992,1993,1995,1998 Gaussian, Inc.
All Rights Reserved.

This is part of the Gaussian(R) 98 program. It is based on
the Gaussian 94(TM) system (copyright 1995 Gaussian, Inc.),
the Gaussian 92(TM) system (copyright 1992 Gaussian, Inc.),
the Gaussian 90(TM) system (copyright 1990 Gaussian, Inc.),
the Gaussian 88(TM) system (copyright 1988 Gaussian, Inc.),
the Gaussian 86(TM) system (copyright 1986 Carnegie Mellon
University), and the Gaussian 82(TM) system (copyright 1983
Carnegie Mellon University). Gaussian is a federally registered
trademark of Gaussian, Inc.

This software contains proprietary and confidential information,
including trade secrets, belonging to Gaussian, Inc.

This software is provided under written license and may be
used, copied, transmitted, or stored only in accord with that
written license.

The following legend is applicable only to US Government
contracts under DFARS:

RESTRICTED RIGHTS LEGEND

Use, duplication or disclosure by the US Government is subject
to restrictions as set forth in subparagraph (c)(1)(ii) of the
Rights in Technical Data and Computer Software clause at DFARS
252.227-7013.

Gaussian, Inc.
Carnegie Office Park, Building 6, Pittsburgh, PA 15106 USA

The following legend is applicable only to US Government
contracts under FAR:

RESTRICTED RIGHTS LEGEND

Use, reproduction and disclosure by the US Government is subject
to restrictions as set forth in subparagraph (c) of the
Commercial Computer Software - Restricted Rights clause at FAR
52.227-19.

Gaussian, Inc.
Carnegie Office Park, Building 6, Pittsburgh, PA 15106 USA

Warning -- This program may not be used in any manner that
competes with the business of Gaussian, Inc. or will provide
assistance to any competitor of Gaussian, Inc. The licensee
of this program is prohibited from giving any competitor of
Gaussian, Inc. access to this program. By using this program,
the user acknowledges that Gaussian, Inc. is engaged in the
business of creating and licensing software in the field of
computational chemistry and represents and warrants to the
licensee that it is not a competitor of Gaussian, Inc. and that
it will not use this program in any manner prohibited above.

Cite this work as:
Gaussian 98, Revision A.11.4,
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria,
M. A. Robb, J. R. Cheeseman, V. G. Zakrzewski, J. A. Montgomery, Jr.,
R. E. Stratmann, J. C. Burant, S. Dapprich, J. M. Millam,
A. D. Daniels, K. N. Kudin, M. C. Strain, O. Farkas, J. Tomasi,
V. Barone, M. Cossi, R. Cammi, B. Mennucci, C. Pomelli, C. Adamo,
S. Clifford, J. Ochterski, G. A. Petersson, P. Y. Ayala, Q. Cui,

K. Morokuma, N. Rega, P. Salvador, J. J. Dannenberg, D. K. Malick,
A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. Cioslowski,
J. V. Ortiz, A. G. Baboul, B. B. Stefanov, G. Liu, A. Liashenko,
P. Piskorz, I. Komaromi, R. Gomperts, R. L. Martin, D. J. Fox,
T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe,
P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, J. L. Andres,
C. Gonzalez, M. Head-Gordon, E. S. Replogle, and J. A. Pople,
Gaussian, Inc., Pittsburgh PA, 2002.

****
Gaussian 98: x86-Win32-G98RevA.11.4 7-May-2002
11-Oct-2015
****
%chk=C:\Users\hp\Desktop\3_cbsqb3.chk
Default route: MaxDisk=2000MB
---
opt freq cbs-qb3 6-311++g(d,p) geom=connectivity

1/14=-1,18=20,26=3,38=1,57=2/1,3;
2/9=110,17=6,18=5,40=1/2;
3/5=4,6=6,7=700,11=2,25=1,30=1/1,2,3;
4//1;
5/5=2,38=4,42=-5/2;
6/7=2,8=2,9=2,10=2,28=1/1;
7//1,2,3,16;
1/14=-1,18=20/3(1);
99//99;
2/9=110/2;
3/5=4,6=6,7=700,11=2,25=1,30=1/1,2,3;
4/5=5,16=2/1;
5/5=2,38=4,42=-5/2;
7//1,2,3,16;
1/14=-1,18=20/3(-5);
2/9=110/2;
6/7=2,8=2,9=2,10=2,19=2,28=1/1;
99/9=1/99;

Title Card Required

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	1.02537	1.59619	0.
H	1.55853	0.66849	0.
H	-0.04463	1.59619	0.
C	-0.28541	-1.25793	0.
H	0.24775	-2.18563	0.
H	-1.35541	-1.25793	0.
C	-1.78647	-4.2389	0.
H	-1.25331	-5.16661	0.
H	-2.85647	-4.2389	0.
O	1.65241	2.68724	0.
O	0.34163	-0.16688	0.
O	-1.15943	-3.14785	0.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Initialization pass.

! Initial Parameters !
! (Angstroms and Degrees) !

! Name	Definition	Value	Derivative Info.	!
! R1	R(1,2)	1.07	estimate D2E/DX2	!
! R2	R(1,3)	1.07	estimate D2E/DX2	!
! R3	R(1,10)	1.2584	estimate D2E/DX2	!
! R4	R(1,11)	1.891	estimate D2E/DX2	!
! R5	R(2,11)	1.476	estimate D2E/DX2	!
! R6	R(3,11)	1.8049	estimate D2E/DX2	!
! R7	R(4,5)	1.07	estimate D2E/DX2	!
! R8	R(4,6)	1.07	estimate D2E/DX2	!
! R9	R(4,11)	1.2584	estimate D2E/DX2	!
! R10	R(4,12)	2.0822	estimate D2E/DX2	!
! R11	R(5,12)	1.7047	estimate D2E/DX2	!

```
! R12   R(6,12)              1.9001       estimate D2E/DX2          !
! R13   R(7,8)               1.07         estimate D2E/DX2          !
! R14   R(7,9)               1.07         estimate D2E/DX2          !
! R15   R(7,12)              1.2584       estimate D2E/DX2          !
! A1    A(2,1,3)            119.8865       estimate D2E/DX2          !
! A2    A(2,1,10)           120.2269       estimate D2E/DX2          !
! A3    A(3,1,10)           119.8865       estimate D2E/DX2          !
! A4    A(10,1,11)          171.3104       estimate D2E/DX2          !
! A5    A(5,4,6)            119.8865       estimate D2E/DX2          !
! A6    A(5,4,11)           120.2269       estimate D2E/DX2          !
! A7    A(6,4,11)           119.8865       estimate D2E/DX2          !
! A8    A(8,7,9)            119.8865       estimate D2E/DX2          !
! A9    A(8,7,12)           120.2269       estimate D2E/DX2          !
! A10   A(9,7,12)           119.8865       estimate D2E/DX2          !
! A11   A(1,11,4)           171.3104       estimate D2E/DX2          !
! A12   A(2,11,3)            67.8889       estimate D2E/DX2          !
! A13   A(2,11,4)           154.3549       estimate D2E/DX2          !
! A14   A(3,11,4)           137.7562       estimate D2E/DX2          !
! A15   A(5,12,6)            61.5564       estimate D2E/DX2          !
! A16   A(5,12,7)           154.2505       estimate D2E/DX2          !
! A17   A(6,12,7)           144.1931       estimate D2E/DX2          !
! A18   L(11,4,12,3,-1)      185.0678       estimate D2E/DX2          !
! A19   L(4,12,7,9,-1)       174.9322       estimate D2E/DX2          !
! A20   L(11,4,12,3,-2)      180.           estimate D2E/DX2          !
! A21   L(4,12,7,9,-2)       180.           estimate D2E/DX2          !
! D1    D(10,1,11,4)         180.           estimate D2E/DX2          !
! D2    D(5,4,11,1)          180.           estimate D2E/DX2          !
! D3    D(5,4,11,2)            0.           estimate D2E/DX2          !
! D4    D(5,4,11,3)          180.           estimate D2E/DX2          !
! D5    D(6,4,11,1)            0.           estimate D2E/DX2          !
! D6    D(6,4,11,2)          180.           estimate D2E/DX2          !
! D7    D(6,4,11,3)            0.           estimate D2E/DX2          !
! D8    D(8,7,11,1)          180.           estimate D2E/DX2          !
! D9    D(8,7,11,2)            0.           estimate D2E/DX2          !
! D10   D(8,7,11,3)          180.           estimate D2E/DX2          !
! D11   D(9,7,11,1)            0.           estimate D2E/DX2          !
! D12   D(9,7,11,2)          180.           estimate D2E/DX2          !
! D13   D(9,7,11,3)            0.           estimate D2E/DX2          !
! D14   D(8,7,12,5)            0.           estimate D2E/DX2          !
! D15   D(8,7,12,6)          180.           estimate D2E/DX2          !
! D16   D(9,7,12,5)          180.           estimate D2E/DX2          !
! D17   D(9,7,12,6)            0.           estimate D2E/DX2          !
--------------------------------------------------------------------------------
Trust Radius=3.00D-01 FncErr=1.00D-07 GrdErr=1.00D-06
Number of steps in this run=  63 maximum allowed number of steps= 100.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

                     Input orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic           Coordinates (Angstroms)
Number     Number      Type             X           Y           Z
---------------------------------------------------------------------
    1          6           0        1.025370    1.596195    0.000000
    2          1           0        1.558534    0.668490    0.000000
    3          1           0       -0.044630    1.596195    0.000000
    4          6           0       -0.285412   -1.257928    0.000000
    5          1           0        0.247751   -2.185633    0.000000
    6          1           0       -1.355412   -1.257928    0.000000
    7          6           0       -1.786469   -4.238901    0.000000
    8          1           0       -1.253306   -5.166606    0.000000
    9          1           0       -2.856469   -4.238901    0.000000
   10          8           0        1.652410    2.687245    0.000000
   11          8           0        0.341628   -0.166878    0.000000
   12          8           0       -1.159429   -3.147850    0.000000
---------------------------------------------------------------------
               Distance matrix (angstroms):
                     1        2        3        4        5
  1  C    0.000000
  2  H    1.070000   0.000000
  3  H    1.070000   1.852234   0.000000
  4  C    3.140727   2.666688   2.864261   0.000000
  5  H    3.860947   3.140727   3.793113   1.070000   0.000000
  6  H    3.716738   3.493160   3.140727   1.070000   1.852234
  7  C    6.477251   5.938984   6.089527   3.337570   2.890322
```

```
  8  H    7.136374   6.477251   6.869961   4.026733   3.337570
  9  H    7.008353   6.601116   6.477251   3.936564   3.721840
 10  O    1.258400   2.020937   2.017508   4.395401   5.071292
 11  O    1.891012   1.476041   1.804888   1.258400   2.020937
 12  O    5.222960   4.685272   4.873268   2.082237   1.704705
                6          7          8          9         10
  6  H    0.000000
  7  C    3.011977   0.000000
  8  H    3.910011   1.070000   0.000000
  9  H    3.337570   1.070000   1.852234   0.000000
 10  O    4.960987   7.732877   8.374136   8.264472   0.000000
 11  O    2.017508   4.594581   5.247961   5.177760   3.140727
 12  O    1.900057   1.258400   2.020937   2.017508   6.477251
               11         12
 11  O    0.000000
 12  O    3.337570   0.000000
Stoichiometry    C3H6O3
Framework group  CS[SG(C3H6O3)]
Deg. of freedom   21
Full point group                 CS     NOp   2
Largest Abelian subgroup         CS     NOp   2
Largest concise Abelian subgroup C1     NOp   1
                         Standard orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic           Coordinates (Angstroms)
Number     Number      Type             X           Y           Z
---------------------------------------------------------------------
   1         6          0       -0.251577   -2.633759    0.000000
   2         1          0        0.672944   -2.095093    0.000000
   3         1          0       -1.179282   -2.100595    0.000000
   4         6          0        0.034120    0.493947    0.000000
   5         1          0        0.958641    1.032613    0.000000
   6         1          0       -0.893585    1.027111    0.000000
   7         6          0        0.218053    3.826444    0.000000
   8         1          0        1.142574    4.365110    0.000000
   9         1          0       -0.709651    4.359608    0.000000
  10         8          0       -0.251577   -3.892159    0.000000
  11         8          0        0.034120   -0.764453    0.000000
  12         8          0        0.218053    2.568044    0.000000
---------------------------------------------------------------------
Rotational constants (GHZ):     93.0213759      0.7531581      0.7471090
Isotopes: C-12,H-1,H-1,C-12,H-1,H-1,C-12,H-1,H-1,O-16,O-16,O-16
Standard basis: CBSB7 (5D, 7F)
There are   108 symmetry adapted basis functions of A'  symmetry.
There are    36 symmetry adapted basis functions of A"  symmetry.
Crude estimate of integral set expansion from redundant integrals=1.000.
Integral buffers will be    262144 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
  144 basis functions      240 primitive gaussians
   24 alpha electrons       24 beta electrons
     nuclear repulsion energy       205.0029143444 Hartrees.
One-electron integrals computed using PRISM.
NBasis=   144 RedAO= T  NBF=   108    36
NBsUse=   144 1.00D-04 NBFU=   108    36
Projected INDO Guess.
Initial guess orbital symmetries:
     Occupied  (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A') (A") (A") (A') (A")
               (A') (A') (A') (A')
     Virtual   (A") (A") (A") (A') (A') (A') (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
               (A") (A") (A") (A") (A") (A") (A") (A") (A") (A")
               (A") (A") (A") (A") (A") (A") (A") (A") (A") (A")
               (A") (A") (A") (A") (A") (A") (A") (A") (A") (A")
Requested convergence on RMS density matrix=1.00D-08 within  64 cycles.
Requested convergence on MAX density matrix=1.00D-06.
```

Integral accuracy reduced to 1.0D-05 until final iterations.
Initial convergence to 1.0D-05 achieved. Increase integral accuracy.
SCF Done: E(RB+HF-LYP) = -343.448974705 A.U. after 14 cycles
Convg = 0.9326D-08 -V/T = 2.0006
S**2 = 0.0000

****

Population analysis using the SCF density.

****

Orbital Symmetries:
Occupied (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
(A') (A') (A') (A') (A') (A') (A") (A') (A") (A')
(A") (A') (A') (A')
Virtual (A") (A") (A") (A') (A') (A') (A') (A') (A') (A')
(A') (A') (A') (A") (A') (A') (A") (A') (A') (A")
(A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
(A") (A') (A") (A") (A") (A') (A') (A") (A') (A")
(A') (A") (A') (A') (A") (A') (A') (A') (A') (A")
(A') (A') (A') (A') (A') (A') (A") (A') (A") (A")
(A") (A') (A') (A") (A") (A') (A') (A') (A') (A')
(A') (A') (A') (A') (A') (A') (A") (A') (A") (A')
(A') (A") (A') (A') (A") (A") (A') (A') (A") (A')
(A") (A') (A") (A') (A") (A') (A') (A') (A') (A')
(A') (A') (A') (A') (A') (A') (A") (A") (A') (A')
(A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
The electronic state is 1-A'.
Alpha occ. eigenvalues -- -19.17462 -19.11438 -19.06078 -10.31487 -10.25087
Alpha occ. eigenvalues -- -10.18256 -1.08811 -1.04231 -0.96395 -0.72375
Alpha occ. eigenvalues -- -0.67856 -0.61439 -0.55116 -0.50997 -0.47025
Alpha occ. eigenvalues -- -0.44857 -0.43831 -0.40995 -0.39225 -0.33263
Alpha occ. eigenvalues -- -0.31815 -0.31057 -0.27113 -0.18743
Alpha virt. eigenvalues -- -0.11766 -0.06191 0.01690 0.01738 0.05798
Alpha virt. eigenvalues -- 0.06696 0.10884 0.11908 0.16119 0.17949
Alpha virt. eigenvalues -- 0.25926 0.27592 0.32192 0.33952 0.36406
Alpha virt. eigenvalues -- 0.37722 0.39727 0.41182 0.42856 0.46879
Alpha virt. eigenvalues -- 0.48373 0.49904 0.51948 0.54346 0.58893
Alpha virt. eigenvalues -- 0.59552 0.62394 0.65082 0.68736 0.74051
Alpha virt. eigenvalues -- 0.76401 0.80129 0.84955 0.96241 0.96688
Alpha virt. eigenvalues -- 0.97100 0.98918 1.01356 1.05826 1.07093
Alpha virt. eigenvalues -- 1.10839 1.18779 1.21957 1.24708 1.28709
Alpha virt. eigenvalues -- 1.34407 1.35730 1.40098 1.40362 1.41188
Alpha virt. eigenvalues -- 1.45935 1.47793 1.52383 1.52995 1.55706
Alpha virt. eigenvalues -- 1.58244 1.68876 1.71447 1.73753 1.78610
Alpha virt. eigenvalues -- 1.84975 1.86944 1.88274 1.89889 1.95765
Alpha virt. eigenvalues -- 1.97775 1.99433 2.12136 2.20612 2.23307
Alpha virt. eigenvalues -- 2.32890 2.40234 2.44373 2.45313 2.48160
Alpha virt. eigenvalues -- 2.50176 2.51208 2.52012 2.57682 2.58426
Alpha virt. eigenvalues -- 2.59314 2.63288 2.63421 2.63940 2.81431
Alpha virt. eigenvalues -- 2.86881 2.87447 2.93184 2.93532 2.99126
Alpha virt. eigenvalues -- 3.19490 3.20343 3.24512 3.26876 3.32921
Alpha virt. eigenvalues -- 3.39733 3.47418 3.48253 3.56538 3.68310
Alpha virt. eigenvalues -- 3.78449 3.85448 3.92480 4.02622 4.11510
Alpha virt. eigenvalues -- 4.76718 4.84934 4.93952 4.98157 4.99569
Alpha virt. eigenvalues -- 5.07879 5.51409 5.60019 5.73112 23.80475
Alpha virt. eigenvalues -- 23.90903 23.94149 49.82362 49.94117 49.99773
Condensed to atoms (all electrons):

		1	2	3	4	5	6
1	C	4.796146	0.432798	0.386050	0.004569	0.001085	-0.001598
2	H	0.432798	0.655576	-0.068463	0.000465	-0.005298	0.001773
3	H	0.386050	-0.068463	0.691818	-0.002418	-0.000181	0.001416
4	C	0.004569	0.000465	-0.002418	4.731829	0.403923	0.376025
5	H	0.001085	-0.005298	-0.000181	0.403923	0.613594	-0.074096
6	H	-0.001598	0.001773	0.001416	0.376025	-0.074096	0.647871
7	C	-0.000001	-0.000006	0.000001	0.004809	0.001364	-0.001281
8	H	0.000000	-0.000001	0.000000	0.000769	-0.003605	0.000581
9	H	0.000000	0.000002	0.000000	-0.000412	0.001586	-0.001199
10	O	0.516245	-0.061047	-0.057399	-0.000238	0.000017	0.000009
11	O	-0.217476	-0.060603	-0.022296	0.464943	-0.047381	-0.044703
12	O	0.000001	0.000028	-0.000013	-0.116620	-0.010943	-0.001609

		7	8	9	10	11	12
1	C	-0.000001	0.000000	0.000000	0.516245	-0.217476	0.000001

```
 2  H   -0.000006  -0.000001   0.000002  -0.061047  -0.060603   0.000028
 3  H    0.000001   0.000000   0.000000  -0.057399  -0.022296  -0.000013
 4  C    0.004809   0.000769  -0.000412  -0.000238   0.464943  -0.116620
 5  H    0.001364  -0.003605   0.001586   0.000017  -0.047381  -0.010943
 6  H   -0.001281   0.000581  -0.001199   0.000009  -0.044703  -0.001609
 7  C    4.613671   0.379460   0.375047   0.000000  -0.000176   0.508943
 8  H    0.379460   0.626462  -0.076163   0.000000   0.000008  -0.044063
 9  H    0.375047  -0.076163   0.632075   0.000000   0.000003  -0.044692
10  O    0.000000   0.000000   0.000000   7.931468   0.005916   0.000000
11  O   -0.000176   0.000008   0.000003   0.005916   8.240275   0.002701
12  O    0.508943  -0.044063  -0.044692   0.000000   0.002701   8.006099
Total atomic charges:
          1
 1  C    0.082179
 2  H    0.104774
 3  H    0.071484
 4  C    0.132356
 5  H    0.119933
 6  H    0.096812
 7  C    0.118169
 8  H    0.116552
 9  H    0.113753
10  O   -0.334972
11  O   -0.321210
12  O   -0.299831
Sum of Mulliken charges=   0.00000
Atomic charges with hydrogens summed into heavy atoms:
          1
 1  C    0.258437
 2  H    0.000000
 3  H    0.000000
 4  C    0.349102
 5  H    0.000000
 6  H    0.000000
 7  C    0.348474
 8  H    0.000000
 9  H    0.000000
10  O   -0.334972
11  O   -0.321210
12  O   -0.299831
Sum of Mulliken charges=   0.00000
Electronic spatial extent (au):  <R**2>=  1384.7146
Charge=     0.0000 electrons
Dipole moment (Debye):
  X=    0.3240   Y=   10.8210   Z=    0.0000  Tot=   10.8258
Quadrupole moment (Debye-Ang):
  XX=   -34.0601   YY=   -38.2290   ZZ=   -34.7210
  XY=    -0.2516   XZ=     0.0000   YZ=     0.0000
Octapole moment (Debye-Ang**2):
 XXX=     1.0956  YYY=   208.1121  ZZZ=     0.0000  XYY=    11.1797
 XXY=     5.0589  XXZ=     0.0000  XZZ=     0.2058  YZZ=    -0.3845
 YYZ=     0.0000  XYZ=     0.0000
Hexadecapole moment (Debye-Ang**3):
XXXX=   -59.0767 YYYY= -1639.9134 ZZZZ=   -29.7648 XXXY=   -52.1503
XXXZ=     0.0000 YYYX=   -58.5309 YYYZ=     0.0000 ZZZX=     0.0000
ZZZY=     0.0000 XXYY=  -268.0749 XXZZ=   -15.7287 YYZZ=  -269.9389
XXYZ=     0.0000 YYXZ=     0.0000 ZZXY=   -17.6394
N-N= 2.050029143444D+02 E-N=-1.218685398161D+03  KE= 3.432502272820D+02
Symmetry A'   KE= 3.323653600180D+02
Symmetry A"   KE= 1.088486726397D+01
***** Axes restored to original set *****
-------------------------------------------------------------------
Center     Atomic                 Forces (Hartrees/Bohr)
Number     Number           X           Y           Z
-------------------------------------------------------------------
   1        6         0.094656025   0.162696099   0.000000000
   2        1         0.036642881   0.031471576   0.000000000
   3        1        -0.011260362   0.017725149   0.000000000
   4        6         0.062031456   0.104646475   0.000000000
   5        1         0.016318040   0.006280881   0.000000000
   6        1        -0.012004129   0.007645340   0.000000000
   7        6         0.040611530   0.071511046   0.000000000
   8        1         0.007749859  -0.018585170   0.000000000
   9        1        -0.020326252  -0.002979980   0.000000000
```

```
 10        8       -0.029406824  -0.036023915   0.000000000
 11        8       -0.108566159  -0.204868237   0.000000000
 12        8       -0.076446068  -0.139519264   0.000000000
---------------------------------------------------------------------
Cartesian Forces:  Max     0.204868237 RMS     0.062878042

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Internal  Forces:  Max     0.095514420 RMS     0.023932769
Search for a local minimum.
Step number   1 out of a maximum of  63
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Second derivative matrix not updated -- first step.
    Eigenvalues ---    0.00230   0.00891   0.01325   0.01534   0.02058
    Eigenvalues ---    0.03565   0.03565   0.06426   0.06445   0.07850
    Eigenvalues ---    0.07985   0.11494   0.12143   0.12958   0.14302
    Eigenvalues ---    0.16000   0.16000   0.18969   0.18972   0.19117
    Eigenvalues ---    0.19162   0.32205   0.32995   0.36606   0.36779
    Eigenvalues ---    0.37230   0.37230   0.80209   0.80209   0.80209
    Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
    Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
    Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
    Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
    Eigenvalues --- 1000.000001000.000001000.00000
RFO step:  Lambda=-1.11811996D-01.
Linear search not attempted -- first point.
Maximum step size (   0.300) exceeded in Quadratic search.
   -- Step size scaled by   0.432
Iteration  1 RMS(Cart)=  0.04760620 RMS(Int)=  0.00044089
Iteration  2 RMS(Cart)=  0.00032739 RMS(Int)=  0.00025646
Iteration  3 RMS(Cart)=  0.00000014 RMS(Int)=  0.00025646
Variable      Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                       (Linear)    (Quad)   (Total)
   R1       2.02201   0.01050   0.00000   0.01337   0.01275   2.03476
   R2       2.02201   0.01347   0.00000   0.01548   0.01499   2.03700
   R3       2.37803  -0.04589   0.00000  -0.02171  -0.02171   2.35632
   R4       3.57349   0.09551   0.00000   0.17875   0.17885   3.75235
   R5       2.78931   0.07051   0.00000   0.13025   0.13052   2.91984
   R6       3.41074   0.03551   0.00000   0.08544   0.08575   3.49649
   R7       2.02201   0.00942   0.00000   0.01147   0.01134   2.03335
   R8       2.02201   0.01331   0.00000   0.01455   0.01445   2.03646
   R9       2.37803  -0.03408   0.00000  -0.01612  -0.01612   2.36191
  R10       3.93486   0.05228   0.00000   0.11204   0.11209   4.04695
  R11       3.22143   0.03201   0.00000   0.07565   0.07570   3.29712
  R12       3.59059   0.02083   0.00000   0.05606   0.05609   3.64668
  R13       2.02201   0.01998   0.00000   0.01784   0.01784   2.03985
  R14       2.02201   0.02033   0.00000   0.01815   0.01815   2.04016
  R15       2.37803  -0.05727   0.00000  -0.02709  -0.02709   2.35094
   A1       2.09241  -0.02752   0.00000  -0.04192  -0.04231   2.05011
   A2       2.09836   0.01640   0.00000   0.02438   0.02470   2.12306
   A3       2.09241   0.01112   0.00000   0.01753   0.01761   2.11002
   A4       2.98993   0.01267   0.00000   0.01630   0.01606   3.00599
   A5       2.09241  -0.01869   0.00000  -0.03052  -0.03057   2.06184
   A6       2.09836   0.01023   0.00000   0.01591   0.01597   2.11432
   A7       2.09241   0.00847   0.00000   0.01461   0.01461   2.10702
   A8       2.09241  -0.00372   0.00000  -0.00592  -0.00592   2.08650
   A9       2.09836   0.00142   0.00000   0.00225   0.00225   2.10061
  A10       2.09241   0.00230   0.00000   0.00367   0.00367   2.09608
  A11       2.98993   0.00128   0.00000   0.00189   0.00152   2.99145
  A12       1.18488  -0.02438   0.00000  -0.05208  -0.05092   1.13397
  A13       2.69400   0.01450   0.00000   0.02995   0.02919   2.72319
  A14       2.40430   0.00988   0.00000   0.02213   0.02173   2.42603
  A15       1.07436  -0.00871   0.00000  -0.02546  -0.02519   1.04917
  A16       2.69218   0.00497   0.00000   0.01377   0.01359   2.70577
  A17       2.51664   0.00375   0.00000   0.01169   0.01160   2.52824
  A18       3.23004  -0.00420   0.00000  -0.00614  -0.00608   3.22396
  A19       3.05314   0.00073   0.00000   0.00098   0.00090   3.05404
  A20       3.14159   0.00000   0.00000   0.00000   0.00000   3.14159
  A21       3.14159   0.00000   0.00000   0.00000   0.00000   3.14159
   D1       3.14159   0.00000   0.00000   0.00000   0.00000   3.14159
   D2       3.14159   0.00000   0.00000   0.00000   0.00000   3.14159
   D3       0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
   D4       3.14159   0.00000   0.00000   0.00000   0.00000   3.14159
   D5       0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
```

D6	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D7	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D8	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D9	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D10	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D11	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D12	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D13	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D14	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D15	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D16	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D17	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

Item	Value	Threshold	Converged?
Maximum Force	0.095514	0.000450	NO
RMS Force	0.023933	0.000300	NO
Maximum Displacement	0.141201	0.001800	NO
RMS Displacement	0.047668	0.001200	NO

Predicted change in Energy=-5.407100D-03
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.130659	2.483583	0.000000
2	1	0	1.658685	1.545193	0.000000
3	1	0	0.053322	2.447774	0.000000
4	6	0	-0.209734	-0.451741	0.000000
5	1	0	0.312476	-1.392527	0.000000
6	1	0	-1.287249	-0.468647	0.000000
7	6	0	-1.742670	-3.467050	0.000000
8	1	0	-1.210760	-4.406339	0.000000
9	1	0	-2.822276	-3.466580	0.000000
10	8	0	1.735017	3.574245	0.000000
11	8	0	0.411883	0.632586	0.000000
12	8	0	-1.118356	-2.390982	0.000000

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	H	1.076748	0.000000			
3	H	1.077932	1.841696	0.000000		
4	C	3.226884	2.734727	2.911423	0.000000	
5	H	3.961521	3.231482	3.849035	1.076003	0.000000
6	H	3.816010	3.568483	3.209772	1.077647	1.847343
7	C	6.608029	6.057375	6.181483	3.382600	2.920149
8	H	7.276899	6.607151	6.969703	4.079326	3.376879
9	H	7.143538	6.722862	6.576370	3.989315	3.758772
10	O	1.246913	2.030487	2.024113	4.471087	5.166473
11	O	1.985656	1.545110	1.850263	1.249869	2.027551
12	O	5.368375	4.817201	4.978593	2.141553	1.744761

		6	7	8	9	10
6	H	0.000000				
7	C	3.032793	0.000000			
8	H	3.938435	1.079440	0.000000		
9	H	3.368073	1.079606	1.865510	0.000000	
10	O	5.047679	7.853288	8.506898	8.387022	0.000000
11	O	2.024787	4.631319	5.293744	5.221393	3.225530
12	O	1.929741	1.244062	2.017474	2.015008	6.612538

		11	12
11	O	0.000000	
12	O	3.388745	0.000000

Stoichiometry C3H6O3
Framework group CS[SG(C3H6O3)]
Deg. of freedom 21
Full point group CS NOp 2
Largest Abelian subgroup CS NOp 2
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	0.010739	-2.725495	0.000000
2	1	0	-0.861475	-2.094124	0.000000
3	1	0	0.974258	-2.242205	0.000000
4	6	0	0.000000	0.501370	0.000000
5	1	0	-0.867935	1.137351	0.000000
6	1	0	0.971589	0.967566	0.000000
7	6	0	0.130673	3.881446	0.000000
8	1	0	-0.745445	4.512008	0.000000
9	1	0	1.111431	4.332735	0.000000
10	8	0	-0.081833	-3.968967	0.000000
11	8	0	-0.110899	-0.743569	0.000000
12	8	0	0.013869	2.642879	0.000000

Rotational constants (GHZ): 92.6816516 0.7256579 0.7200205
Isotopes: C-12,H-1,H-1,C-12,H-1,H-1,C-12,H-1,H-1,O-16,O-16,O-16
Standard basis: CBSB7 (5D, 7F)
There are 108 symmetry adapted basis functions of A' symmetry.
There are 36 symmetry adapted basis functions of A" symmetry.
Crude estimate of integral set expansion from redundant integrals=1.000.
Integral buffers will be 262144 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
144 basis functions 240 primitive gaussians
24 alpha electrons 24 beta electrons
nuclear repulsion energy 202.6932879941 Hartrees.
One-electron integrals computed using PRISM.
NBasis= 144 RedAO= T NBF= 108 36
NBsUse= 144 1.00D-04 NBFU= 108 36
Initial guess read from the read-write file:
Initial guess orbital symmetries:
Occupied (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
(A') (A') (A') (A') (A') (A') (A") (A') (A") (A')
(A") (A') (A') (A')
Virtual (A") (A") (A") (A') (A') (A') (A') (A') (A') (A')
(A') (A') (A') (A") (A') (A') (A") (A') (A') (A")
(A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
(A") (A') (A") (A") (A") (A') (A') (A") (A') (A")
(A') (A") (A') (A') (A") (A') (A') (A') (A') (A")
(A') (A') (A') (A') (A') (A') (A") (A') (A") (A")
(A") (A') (A') (A") (A") (A') (A') (A') (A') (A')
(A') (A') (A') (A') (A') (A') (A") (A') (A") (A')
(A') (A") (A') (A') (A") (A") (A') (A') (A") (A')
(A") (A') (A") (A') (A") (A') (A') (A') (A') (A')
(A') (A') (A') (A') (A') (A") (A") (A") (A') (A')
(A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
Requested convergence on RMS density matrix=1.00D-08 within 64 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Integral accuracy reduced to 1.0D-05 until final iterations.
Initial convergence to 1.0D-05 achieved. Increase integral accuracy.
SCF Done: E(RB+HF-LYP) = -343.491808528 A.U. after 17 cycles
Convg = 0.3764D-08 -V/T = 2.0011
S**2 = 0.0000
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.072760538	0.127488550	0.000000000
2	1	0.027378063	0.025676272	0.000000000
3	1	-0.007991220	0.014135019	0.000000000
4	6	0.052950951	0.089107888	0.000000000
5	1	0.014019626	0.006674606	0.000000000
6	1	-0.008021966	0.007535616	0.000000000
7	6	0.031483615	0.054748329	0.000000000
8	1	0.004423337	-0.013777791	0.000000000
9	1	-0.014349529	-0.003203241	0.000000000
10	8	-0.023913593	-0.032543170	0.000000000
11	8	-0.086307589	-0.163027336	0.000000000
12	8	-0.062432232	-0.112814743	0.000000000

Cartesian Forces: Max 0.163027336 RMS 0.050283395

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.

Internal Forces: Max 0.072356978 RMS 0.018825949
Search for a local minimum.
Step number 2 out of a maximum of 63
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Update second derivatives using information from points 1 2
Trust test= 7.92D+00 RLast= 3.00D-01 DXMaxT set to 4.24D-01
Maximum step size (0.424) exceeded in linear search.
-- Step size scaled by 0.707
Quartic linear search produced a step of 1.41429.
Iteration 1 RMS(Cart)= 0.06234607 RMS(Int)= 0.00569872
Iteration 2 RMS(Cart)= 0.00580932 RMS(Int)= 0.00081339
Iteration 3 RMS(Cart)= 0.00001198 RMS(Int)= 0.00081326
Iteration 4 RMS(Cart)= 0.00000001 RMS(Int)= 0.00081326

Variable	Old X	-DE/DX (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.03476	0.00696	0.01804	0.00000	0.01622	2.05098
R2	2.03700	0.01023	0.02120	0.00000	0.01973	2.05673
R3	2.35632	-0.04006	-0.03070	0.00000	-0.03070	2.32562
R4	3.75235	0.07236	0.25295	0.00000	0.25314	4.00548
R5	2.91984	0.05388	0.18460	0.00000	0.18543	3.10526
R6	3.49649	0.02784	0.12127	0.00000	0.12221	3.61870
R7	2.03335	0.00726	0.01604	0.00000	0.01564	2.04899
R8	2.03646	0.00962	0.02044	0.00000	0.02011	2.05657
R9	2.36191	-0.03352	-0.02280	0.00000	-0.02280	2.33911
R10	4.04695	0.04309	0.15853	0.00000	0.15867	4.20562
R11	3.29712	0.02717	0.10706	0.00000	0.10720	3.40432
R12	3.64668	0.01781	0.07933	0.00000	0.07944	3.72612
R13	2.03985	0.01417	0.02523	0.00000	0.02523	2.06508
R14	2.04016	0.01435	0.02567	0.00000	0.02567	2.06583
R15	2.35094	-0.04349	-0.03832	0.00000	-0.03832	2.31262
A1	2.05011	-0.02047	-0.05984	0.00000	-0.06119	1.98892
A2	2.12306	0.01190	0.03493	0.00000	0.03596	2.15902
A3	2.11002	0.00857	0.02490	0.00000	0.02522	2.13525
A4	3.00599	0.00879	0.02271	0.00000	0.02199	3.02798
A5	2.06184	-0.01457	-0.04324	0.00000	-0.04344	2.01840
A6	2.11432	0.00813	0.02258	0.00000	0.02278	2.13710
A7	2.10702	0.00644	0.02066	0.00000	0.02066	2.12768
A8	2.08650	-0.00418	-0.00837	0.00000	-0.00837	2.07812
A9	2.10061	0.00181	0.00319	0.00000	0.00319	2.10380
A10	2.09608	0.00237	0.00518	0.00000	0.00518	2.10127
A11	2.99145	0.00111	0.00215	0.00000	0.00103	2.99248
A12	1.13397	-0.01780	-0.07201	0.00000	-0.06828	1.06568
A13	2.72319	0.01013	0.04128	0.00000	0.03885	2.76204
A14	2.42603	0.00768	0.03074	0.00000	0.02943	2.45546
A15	1.04917	-0.00754	-0.03563	0.00000	-0.03474	1.01443
A16	2.70577	0.00411	0.01923	0.00000	0.01866	2.72443
A17	2.52824	0.00342	0.01640	0.00000	0.01609	2.54433
A18	3.22396	-0.00348	-0.00860	0.00000	-0.00840	3.21556
A19	3.05404	0.00052	0.00127	0.00000	0.00102	3.05506
A20	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
A21	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D1	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D2	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D4	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D5	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D6	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D7	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D8	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D9	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D10	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D11	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D12	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D13	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D14	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D15	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D16	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D17	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

Item	Value	Threshold	Converged?
Maximum Force	0.072357	0.000450	NO
RMS Force	0.018826	0.000300	NO
Maximum Displacement	0.200506	0.001800	NO
RMS Displacement	0.067418	0.001200	NO

Predicted change in Energy=-1.067803D-02

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.181295	2.586052	0.000000
2	1	0	1.700595	1.633016	0.000000
3	1	0	0.096471	2.498221	0.000000
4	6	0	-0.199428	-0.464784	0.000000
5	1	0	0.306383	-1.423856	0.000000
6	1	0	-1.286945	-0.505827	0.000000
7	6	0	-1.778303	-3.528192	0.000000
8	1	0	-1.248583	-4.484011	0.000000
9	1	0	-2.871493	-3.526813	0.000000
10	8	0	1.753585	3.675560	0.000000
11	8	0	0.414713	0.609919	0.000000
12	8	0	-1.157813	-2.473374	0.000000

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	H	1.085334	0.000000			
3	H	1.088374	1.822579	0.000000		
4	C	3.348731	2.830345	2.977743	0.000000	
5	H	4.104246	3.359805	3.927690	1.084281	0.000000
6	H	3.956252	3.674241	3.307287	1.088291	1.838878
7	C	6.792879	6.224211	6.311294	3.446348	2.962119
8	H	7.475968	6.790852	7.110607	4.153903	3.432560
9	H	7.334318	6.894043	6.716387	4.063982	3.810686
10	O	1.230667	2.043231	2.032769	4.577849	5.300795
11	O	2.119611	1.643235	1.914932	1.237803	2.036658
12	O	5.573977	5.003293	5.127376	2.225519	1.801488

		6	7	8	9	10
6	H	0.000000				
7	C	3.062046	0.000000			
8	H	3.978369	1.092791	0.000000		
9	H	3.411327	1.093191	1.884161	0.000000	
10	O	5.169992	8.022984	8.694343	8.559528	0.000000
11	O	2.034829	4.683298	5.358607	5.283153	3.345255
12	O	1.971780	1.223785	2.012685	2.011575	6.803354

		11	12
11	O	0.000000	
12	O	3.461146	0.000000

Stoichiometry C3H6O3
Framework group CS[SG(C3H6O3)]
Deg. of freedom 21
Full point group CS NOp 2
Largest Abelian subgroup CS NOp 2
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.078914	-2.837311	0.000000
2	1	0	-0.929311	-2.162941	0.000000
3	1	0	0.885355	-2.332589	0.000000
4	6	0	0.000000	0.510491	0.000000
5	1	0	-0.840340	1.195686	0.000000
6	1	0	0.985029	0.973195	0.000000
7	6	0	0.256401	3.947287	0.000000
8	1	0	-0.604676	4.620147	0.000000
9	1	0	1.263227	4.373159	0.000000
10	8	0	-0.180007	-4.063818	0.000000
11	8	0	-0.145403	-0.718742	0.000000
12	8	0	0.097384	2.733878	0.000000

Rotational constants (GHZ): 91.8966078 0.6892284 0.6840977
Isotopes: C-12,H-1,H-1,C-12,H-1,H-1,C-12,H-1,H-1,O-16,O-16,O-16
Standard basis: CBSB7 (5D, 7F)
There are 108 symmetry adapted basis functions of A' symmetry.
There are 36 symmetry adapted basis functions of A" symmetry.

Crude estimate of integral set expansion from redundant integrals=1.000.
Integral buffers will be 262144 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
144 basis functions 240 primitive gaussians
24 alpha electrons 24 beta electrons
nuclear repulsion energy 199.7155912854 Hartrees.
One-electron integrals computed using PRISM.
NBasis= 144 RedAO= T NBF= 108 36
NBsUse= 144 1.00D-04 NBFU= 108 36
Initial guess read from the read-write file:
Initial guess orbital symmetries:
Occupied (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
(A') (A') (A') (A') (A') (A') (A") (A') (A") (A')
(A") (A') (A') (A')
Virtual (A") (A") (A") (A') (A') (A') (A') (A') (A') (A')
(A') (A') (A') (A") (A') (A') (A") (A') (A') (A")
(A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
(A") (A') (A") (A") (A") (A') (A') (A") (A') (A")
(A') (A') (A") (A') (A") (A') (A') (A") (A') (A')
(A') (A') (A') (A') (A') (A') (A') (A") (A') (A")
(A") (A') (A') (A") (A") (A') (A') (A') (A') (A')
(A') (A') (A') (A') (A') (A') (A') (A") (A') (A")
(A') (A') (A") (A') (A") (A") (A') (A") (A') (A')
(A") (A') (A") (A') (A") (A') (A') (A') (A') (A')
(A') (A') (A') (A') (A') (A") (A") (A") (A') (A')
(A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
Requested convergence on RMS density matrix=1.00D-08 within 64 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Integral accuracy reduced to 1.0D-05 until final iterations.
Initial convergence to 1.0D-05 achieved. Increase integral accuracy.
SCF Done: E(RB+HF-LYP) = -343.536036000 A.U. after 12 cycles
Convg = 0.3946D-08 -V/T = 2.0017
S**2 = 0.0000
***** Axes restored to original set *****

Center Atomic Forces (Hartrees/Bohr)
Number Number X Y Z
---
1 6 0.044547688 0.082850662 0.000000000
2 1 0.020234097 0.019573347 0.000000000
3 1 -0.004772539 0.011893134 0.000000000
4 6 0.038861391 0.066556189 0.000000000
5 1 0.011974652 0.007597765 0.000000000
6 1 -0.003129927 0.008106523 0.000000000
7 6 0.016841259 0.028720068 0.000000000
8 1 0.000151240 -0.007536248 0.000000000
9 1 -0.006640739 -0.003576200 0.000000000
10 8 -0.015134167 -0.023639161 0.000000000
11 8 -0.060676865 -0.114957069 0.000000000
12 8 -0.042256088 -0.075589009 0.000000000

Cartesian Forces: Max 0.114957069 RMS 0.034330164

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Internal Forces: Max 0.046664637 RMS 0.012658008
Search for a local minimum.
Step number 3 out of a maximum of 63
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Update second derivatives using information from points 2 3
Maximum step size (0.424) exceeded in linear search.
-- Step size scaled by 0.500
Quartic linear search produced a step of 1.00020.
Iteration 1 RMS(Cart)= 0.06232429 RMS(Int)= 0.00571167
Iteration 2 RMS(Cart)= 0.00581261 RMS(Int)= 0.00084914
Iteration 3 RMS(Cart)= 0.00001201 RMS(Int)= 0.00084902
Iteration 4 RMS(Cart)= 0.00000001 RMS(Int)= 0.00084902
Variable Old X -DE/DX Delta X Delta X Delta X New X
(Linear) (Quad) (Total)
R1 2.05098 0.00410 0.01623 0.00000 0.01451 2.06549
R2 2.05673 0.00643 0.01974 0.00000 0.01830 2.07502
R3 2.32562 -0.02797 -0.03071 0.00000 -0.03071 2.29492
R4 4.00548 0.04666 0.25319 0.00000 0.25319 4.25867

R5	3.10526	0.03707	0.18547	0.00000	0.18634	3.29160
R6	3.61870	0.02000	0.12223	0.00000	0.12322	3.74191
R7	2.04899	0.00454	0.01564	0.00000	0.01523	2.06422
R8	2.05657	0.00489	0.02012	0.00000	0.01977	2.07635
R9	2.33911	-0.02892	-0.02281	0.00000	-0.02281	2.31630
R10	4.20562	0.03180	0.15870	0.00000	0.15883	4.36445
R11	3.40432	0.02175	0.10722	0.00000	0.10738	3.51170
R12	3.72612	0.01454	0.07946	0.00000	0.07958	3.80571
R13	2.06508	0.00667	0.02524	0.00000	0.02524	2.09031
R14	2.06583	0.00663	0.02568	0.00000	0.02568	2.09151
R15	2.31262	-0.02043	-0.03833	0.00000	-0.03833	2.27429
A1	1.98892	-0.01132	-0.06120	0.00000	-0.06276	1.92617
A2	2.15902	0.00606	0.03597	0.00000	0.03707	2.19609
A3	2.13525	0.00527	0.02523	0.00000	0.02568	2.16093
A4	3.02798	0.00481	0.02200	0.00000	0.02135	3.04933
A5	2.01840	-0.00919	-0.04345	0.00000	-0.04370	1.97470
A6	2.13710	0.00524	0.02279	0.00000	0.02302	2.16012
A7	2.12768	0.00395	0.02067	0.00000	0.02069	2.14837
A8	2.07812	-0.00489	-0.00837	0.00000	-0.00837	2.06975
A9	2.10380	0.00237	0.00319	0.00000	0.00319	2.10698
A10	2.10127	0.00252	0.00519	0.00000	0.00519	2.10645
A11	2.99248	0.00073	0.00103	0.00000	-0.00009	2.99239
A12	1.06568	-0.01075	-0.06829	0.00000	-0.06435	1.00133
A13	2.76204	0.00569	0.03886	0.00000	0.03633	2.79837
A14	2.45546	0.00506	0.02944	0.00000	0.02803	2.48349
A15	1.01443	-0.00617	-0.03475	0.00000	-0.03378	0.98065
A16	2.72443	0.00314	0.01866	0.00000	0.01804	2.74247
A17	2.54433	0.00303	0.01609	0.00000	0.01574	2.56007
A18	3.21556	-0.00254	-0.00840	0.00000	-0.00819	3.20737
A19	3.05506	0.00027	0.00102	0.00000	0.00074	3.05580
A20	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
A21	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D1	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D2	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D4	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D5	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D6	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D7	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D8	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D9	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D10	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D11	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D12	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D13	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D14	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D15	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D16	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D17	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

Item	Value	Threshold	Converged?
Maximum Force	0.046665	0.000450	NO
RMS Force	0.012658	0.000300	NO
Maximum Displacement	0.201337	0.001800	NO
RMS Displacement	0.067403	0.001200	NO

Predicted change in Energy=-8.649513D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.230917	2.687470	0.000000
2	1	0	1.739984	1.720245	0.000000
3	1	0	0.142001	2.546093	0.000000
4	6	0	-0.188275	-0.479585	0.000000
5	1	0	0.300102	-1.456667	0.000000
6	1	0	-1.285079	-0.545045	0.000000
7	6	0	-1.814074	-3.590535	0.000000
8	1	0	-1.287031	-4.563048	0.000000
9	1	0	-2.920850	-3.587966	0.000000
10	8	0	1.771164	3.775102	0.000000
11	8	0	0.418596	0.585371	0.000000
12	8	0	-1.197401	-2.557030	0.000000

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	H	1.093011	0.000000			
3	H	1.098055	1.798770	0.000000		
4	C	3.470496	2.925310	3.043651	0.000000	
5	H	4.247386	3.487984	4.005881	1.092338	0.000000
6	H	4.096266	3.779226	3.404658	1.098756	1.828621
7	C	6.977486	6.390283	6.440841	3.510161	3.003853
8	H	7.675290	6.974425	7.251346	4.228704	3.488351
9	H	7.524511	7.064028	6.856219	4.138719	3.862249
10	O	1.214418	2.055093	2.040744	4.684204	5.434651
11	O	2.253593	1.741840	1.980135	1.225735	2.045474
12	O	5.779403	5.188768	5.275970	2.309569	1.858309

		6	7	8	9	10
6	H	0.000000				
7	C	3.091091	0.000000			
8	H	4.018003	1.106145	0.000000		
9	H	3.454723	1.106779	1.902669	0.000000	
10	O	5.291908	8.191858	8.881290	8.730966	0.000000
11	O	2.044591	4.735294	5.423596	5.344965	3.464653
12	O	2.013894	1.203503	2.008020	2.008260	6.993445

		11	12
11	O	0.000000	
12	O	3.533572	0.000000

Stoichiometry C3H6O3
Framework group CS[SG(C3H6O3)]
Deg. of freedom 21
Full point group CS NOp 2
Largest Abelian subgroup CS NOp 2
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.176232	-2.946046	0.000000
2	1	0	-1.000957	-2.228758	0.000000
3	1	0	0.787618	-2.420005	0.000000
4	6	0	0.000000	0.519973	0.000000
5	1	0	-0.809008	1.253940	0.000000
6	1	0	0.998689	0.978104	0.000000
7	6	0	0.389135	4.008498	0.000000
8	1	0	-0.454262	4.724207	0.000000
9	1	0	1.421750	4.406826	0.000000
10	8	0	-0.286034	-4.155489	0.000000
11	8	0	-0.180116	-0.692456	0.000000
12	8	0	0.188494	2.821837	0.000000

Rotational constants (GHZ): 90.7060688 0.6554629 0.6507603
Isotopes: C-12,H-1,H-1,C-12,H-1,H-1,C-12,H-1,H-1,O-16,O-16,O-16
Standard basis: CBSB7 (5D, 7F)
There are 108 symmetry adapted basis functions of A' symmetry.
There are 36 symmetry adapted basis functions of A" symmetry.
Crude estimate of integral set expansion from redundant integrals=1.000.
Integral buffers will be 262144 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
144 basis functions 240 primitive gaussians
24 alpha electrons 24 beta electrons
nuclear repulsion energy 197.0413953158 Hartrees.
One-electron integrals computed using PRISM.
NBasis= 144 RedAO= T NBF= 108 36
NBsUse= 144 1.00D-04 NBFU= 108 36
Initial guess read from the read-write file:
Initial guess orbital symmetries:
Occupied (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
(A') (A') (A') (A') (A') (A') (A") (A') (A") (A')
(A") (A') (A') (A')
Virtual (A") (A") (A") (A') (A') (A') (A') (A') (A') (A')
(A') (A') (A') (A") (A') (A') (A") (A') (A') (A')
(A") (A') (A') (A') (A') (A') (A') (A') (A') (A')
(A") (A') (A") (A") (A') (A") (A') (A') (A") (A")

(A') (A') (A") (A') (A") (A') (A") (A') (A') (A')
(A') (A') (A') (A') (A') (A') (A") (A') (A") (A")
(A') (A') (A") (A") (A") (A') (A') (A') (A') (A')
(A') (A') (A') (A') (A') (A') (A') (A") (A') (A')
(A") (A') (A") (A') (A") (A") (A') (A") (A') (A')
(A") (A") (A') (A') (A") (A') (A') (A') (A') (A')
(A') (A') (A') (A') (A') (A") (A") (A") (A') (A')
(A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
Requested convergence on RMS density matrix=1.00D-08 within 64 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Integral accuracy reduced to 1.0D-05 until final iterations.
Initial convergence to 1.0D-05 achieved. Increase integral accuracy.
SCF Done: E(RB+HF-LYP) = -343.564907586 A.U. after 11 cycles
Convg = 0.8292D-08 -V/T = 2.0020
S**2 = 0.0000
***** Axes restored to original set *****

Center Atomic Forces (Hartrees/Bohr)
Number Number X Y Z
---
1 6 0.019378190 0.042442115 0.000000000
2 1 0.017836093 0.015655320 0.000000000
3 1 -0.002859876 0.012176968 0.000000000
4 6 0.023981618 0.043536250 0.000000000
5 1 0.011139041 0.008890146 0.000000000
6 1 0.000991054 0.009397855 0.000000000
7 6 0.000029224 -0.000188606 0.000000000
8 1 -0.003637494 -0.001912821 0.000000000
9 1 0.000241923 -0.003998961 0.000000000
10 8 -0.005485423 -0.010593025 0.000000000
11 8 -0.040327396 -0.077129562 0.000000000
12 8 -0.021286954 -0.038275678 0.000000000

Cartesian Forces: Max 0.077129562 RMS 0.020634496

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Internal Forces: Max 0.027556961 RMS 0.008084744
Search for a local minimum.
Step number 4 out of a maximum of 63
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Update second derivatives using information from points 3 4
Maximum step size (0.424) exceeded in linear search.
-- Step size scaled by 0.500
Quartic linear search produced a step of 1.00020.
Iteration 1 RMS(Cart)= 0.06229862 RMS(Int)= 0.00568558
Iteration 2 RMS(Cart)= 0.00579332 RMS(Int)= 0.00075130
Iteration 3 RMS(Cart)= 0.00001207 RMS(Int)= 0.00075117
Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00075117
Variable Old X -DE/DX Delta X Delta X Delta X New X
(Linear) (Quad) (Total)
R1 2.06549 0.00274 0.01451 0.00000 0.01314 2.07864
R2 2.07502 0.00341 0.01830 0.00000 0.01712 2.09215
R3 2.29492 -0.01193 -0.03071 0.00000 -0.03071 2.26420
R4 4.25867 0.02756 0.25324 0.00000 0.25303 4.51171
R5 3.29160 0.02618 0.18637 0.00000 0.18717 3.47877
R6 3.74191 0.01505 0.12324 0.00000 0.12414 3.86605
R7 2.06422 0.00213 0.01523 0.00000 0.01486 2.07908
R8 2.07635 0.00068 0.01978 0.00000 0.01947 2.09582
R9 2.31630 -0.02083 -0.02281 0.00000 -0.02281 2.29349
R10 4.36445 0.02221 0.15886 0.00000 0.15895 4.52340
R11 3.51170 0.01779 0.10740 0.00000 0.10755 3.61924
R12 3.80571 0.01226 0.07960 0.00000 0.07972 3.88543
R13 2.09031 -0.00005 0.02524 0.00000 0.02524 2.11555
R14 2.09151 -0.00025 0.02568 0.00000 0.02568 2.11719
R15 2.27429 0.00696 -0.03833 0.00000 -0.03833 2.23596
A1 1.92617 -0.00312 -0.06277 0.00000 -0.06429 1.86188
A2 2.19609 0.00078 0.03708 0.00000 0.03808 2.23417
A3 2.16093 0.00234 0.02569 0.00000 0.02621 2.18714
A4 3.04933 0.00203 0.02135 0.00000 0.02088 3.07021
A5 1.97470 -0.00424 -0.04371 0.00000 -0.04397 1.93073
A6 2.16012 0.00244 0.02302 0.00000 0.02324 2.18336
A7 2.14837 0.00179 0.02069 0.00000 0.02073 2.16910
A8 2.06975 -0.00565 -0.00837 0.00000 -0.00837 2.06138

A9	2.10698	0.00293	0.00319	0.00000	0.00319	2.11017
A10	2.10645	0.00272	0.00519	0.00000	0.00519	2.11164
A11	2.99239	0.00035	-0.00009	0.00000	-0.00103	2.99136
A12	1.00133	-0.00562	-0.06437	0.00000	-0.06087	0.94046
A13	2.79837	0.00263	0.03634	0.00000	0.03412	2.83248
A14	2.48349	0.00300	0.02803	0.00000	0.02675	2.51024
A15	0.98065	-0.00505	-0.03379	0.00000	-0.03289	0.94775
A16	2.74247	0.00238	0.01805	0.00000	0.01747	2.75995
A17	2.56007	0.00267	0.01574	0.00000	0.01542	2.57549
A18	3.20737	-0.00171	-0.00820	0.00000	-0.00802	3.19935
A19	3.05580	0.00004	0.00074	0.00000	0.00050	3.05630
A20	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
A21	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D1	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D2	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D4	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D5	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D6	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D7	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D8	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D9	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D10	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D11	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D12	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D13	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D14	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D15	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D16	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D17	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

Item	Value	Threshold	Converged?
Maximum Force	0.027557	0.000450	NO
RMS Force	0.008085	0.000300	NO
Maximum Displacement	0.202016	0.001800	NO
RMS Displacement	0.067363	0.001200	NO

Predicted change in Energy=-6.799648D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.279493	2.789263	0.000000
2	1	0	1.777030	1.808251	0.000000
3	1	0	0.189924	2.592925	0.000000
4	6	0	-0.176242	-0.494620	0.000000
5	1	0	0.293700	-1.489407	0.000000
6	1	0	-1.281630	-0.584790	0.000000
7	6	0	-1.849925	-3.652531	0.000000
8	1	0	-1.326045	-4.641891	0.000000
9	1	0	-2.970287	-3.648498	0.000000
10	8	0	1.787730	3.874295	0.000000
11	8	0	0.423543	0.560481	0.000000
12	8	0	-1.237088	-2.640388	0.000000

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	H	1.099967	0.000000			
3	H	1.107117	1.770485	0.000000		
4	C	3.592081	3.019683	3.109182	0.000000	
5	H	4.390763	3.615911	4.083651	1.100202	0.000000
6	H	4.235987	3.883561	3.501906	1.109060	1.816589
7	C	7.161701	6.555528	6.570138	3.574020	3.045363
8	H	7.874698	7.157752	7.391937	4.303708	3.544253
9	H	7.713974	7.232781	6.995877	4.213506	3.913475
10	O	1.198165	2.066071	2.048143	4.790052	5.567892
11	O	2.387492	1.840885	2.045827	1.213664	2.053996
12	O	5.984504	5.373574	5.424383	2.393682	1.915221

		6	7	8	9	10
6	H	0.000000				
7	C	3.119935	0.000000			
8	H	4.057344	1.119502	0.000000		

```
   9  H    3.498266   1.120369   1.921032   0.000000
  10  O    5.413354   8.359763   9.067580   8.901187   0.000000
  11  O    2.054084   4.787288   5.488691   5.406809   3.583625
  12  O    2.056080   1.183217   2.003479   2.005059   7.182661
             11         12
  11  O    0.000000
  12  O    3.606003   0.000000
Stoichiometry    C3H6O3
Framework group  CS[SG(C3H6O3)]
Deg. of freedom   21
Full point group                 CS     NOp   2
Largest Abelian subgroup         CS     NOp   2
Largest concise Abelian subgroup C1     NOp   1
                    Standard orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic           Coordinates (Angstroms)
Number     Number      Type             X           Y           Z
---------------------------------------------------------------------
   1         6           0      -0.281124   -3.051211    0.000000
   2         1           0      -1.076517   -2.291423    0.000000
   3         1           0       0.681186   -2.503792    0.000000
   4         6           0       0.000000    0.529852    0.000000
   5         1           0      -0.773947    1.311806    0.000000
   6         1           0       1.012527    0.982403    0.000000
   7         6           0       0.528556    4.064573    0.000000
   8         1           0      -0.294456    4.823476    0.000000
   9         1           0       1.586526    4.433257    0.000000
  10         8           0      -0.399706   -4.243494    0.000000
  11         8           0      -0.214874   -0.664639    0.000000
  12         8           0       0.287091    2.906256    0.000000
---------------------------------------------------------------------
Rotational constants (GHZ):     89.0688230      0.6241396      0.6197965
Isotopes: C-12,H-1,H-1,C-12,H-1,H-1,C-12,H-1,H-1,O-16,O-16,O-16
Standard basis: CBSB7 (5D, 7F)
There are   108 symmetry adapted basis functions of A'  symmetry.
There are    36 symmetry adapted basis functions of A"  symmetry.
Crude estimate of integral set expansion from redundant integrals=1.000.
Integral buffers will be    262144 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
  144 basis functions     240 primitive gaussians
   24 alpha electrons      24 beta electrons
     nuclear repulsion energy       194.6389410356 Hartrees.
One-electron integrals computed using PRISM.
NBasis=   144 RedAO= T  NBF=   108    36
NBsUse=   144 1.00D-04 NBFU=   108    36
Initial guess read from the read-write file:
Initial guess orbital symmetries:
     Occupied  (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A') (A") (A') (A") (A')
               (A") (A') (A') (A')
     Virtual   (A") (A") (A") (A') (A') (A') (A') (A') (A') (A')
               (A') (A') (A') (A") (A') (A') (A") (A') (A') (A')
               (A") (A') (A') (A') (A') (A') (A') (A') (A') (A')
               (A') (A") (A") (A") (A') (A') (A") (A') (A") (A')
               (A") (A') (A") (A') (A") (A") (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A') (A') (A") (A") (A')
               (A') (A") (A") (A") (A") (A') (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A') (A') (A') (A") (A')
               (A") (A') (A") (A') (A") (A") (A') (A") (A') (A')
               (A") (A") (A') (A") (A') (A') (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A") (A") (A") (A') (A')
               (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
Requested convergence on RMS density matrix=1.00D-08 within  64 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Integral accuracy reduced to 1.0D-05 until final iterations.
Initial convergence to 1.0D-05 achieved.  Increase integral accuracy.
SCF Done:  E(RB+HF-LYP) =  -343.581574310     A.U. after   11 cycles
          Convg  =    0.7689D-08           -V/T =  2.0021
          S**2   =   0.0000
***** Axes restored to original set *****
---------------------------------------------------------------------
Center     Atomic              Forces (Hartrees/Bohr)
Number     Number           X           Y           Z
```

1	6	-0.003245173	0.004110892	0.000000000
2	1	0.018645703	0.013494418	0.000000000
3	1	-0.002130404	0.014293322	0.000000000
4	6	0.008687392	0.020086705	0.000000000
5	1	0.011293046	0.010442532	0.000000000
6	1	0.004457063	0.011329441	0.000000000
7	6	-0.019180028	-0.032222896	0.000000000
8	1	-0.006970067	0.003110862	0.000000000
9	1	0.006342440	-0.004454688	0.000000000
10	8	0.004788789	0.006369591	0.000000000
11	8	-0.023643990	-0.046496873	0.000000000
12	8	0.000955229	-0.000063306	0.000000000

Cartesian Forces: Max 0.046496873 RMS 0.012844923

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Internal Forces: Max 0.038972596 RMS 0.007703984
Search for a local minimum.
Step number 5 out of a maximum of 63
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Update second derivatives using information from points 4 5
Maximum step size (0.424) exceeded in linear search.
-- Step size scaled by 0.762
Quartic linear search produced a step of 1.00016.
Iteration 1 RMS(Cart)= 0.06227643 RMS(Int)= 0.00563872
Iteration 2 RMS(Cart)= 0.00574671 RMS(Int)= 0.00066970
Iteration 3 RMS(Cart)= 0.00001207 RMS(Int)= 0.00066957
Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00066957

Variable	Old X	-DE/DX (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.07864	0.00229	0.01315	0.00000	0.01208	2.09071
R2	2.09215	0.00110	0.01713	0.00000	0.01619	2.10834
R3	2.26420	0.00780	-0.03072	0.00000	-0.03072	2.23349
R4	4.51171	0.01323	0.25307	0.00000	0.25268	4.76439
R5	3.47877	0.01953	0.18720	0.00000	0.18794	3.66671
R6	3.86605	0.01224	0.12416	0.00000	0.12500	3.99105
R7	2.07908	0.00000	0.01486	0.00000	0.01454	2.09362
R8	2.09582	-0.00307	0.01948	0.00000	0.01920	2.11502
R9	2.29349	-0.00991	-0.02281	0.00000	-0.02281	2.27068
R10	4.52340	0.01402	0.15898	0.00000	0.15902	4.68243
R11	3.61924	0.01503	0.10756	0.00000	0.10771	3.72695
R12	3.88543	0.01079	0.07973	0.00000	0.07986	3.96529
R13	2.11555	-0.00601	0.02524	0.00000	0.02524	2.14080
R14	2.11719	-0.00636	0.02569	0.00000	0.02569	2.14288
R15	2.23596	0.03897	-0.03834	0.00000	-0.03834	2.19762
A1	1.86188	0.00443	-0.06430	0.00000	-0.06578	1.79610
A2	2.23417	-0.00409	0.03808	0.00000	0.03899	2.27316
A3	2.18714	-0.00034	0.02621	0.00000	0.02680	2.21393
A4	3.07021	0.00006	0.02089	0.00000	0.02057	3.09078
A5	1.93073	0.00037	-0.04397	0.00000	-0.04424	1.88649
A6	2.18336	-0.00020	0.02324	0.00000	0.02345	2.20681
A7	2.16910	-0.00016	0.02073	0.00000	0.02079	2.18988
A8	2.06138	-0.00644	-0.00838	0.00000	-0.00838	2.05300
A9	2.11017	0.00351	0.00319	0.00000	0.00319	2.11336
A10	2.11164	0.00294	0.00519	0.00000	0.00519	2.11683
A11	2.99136	-0.00003	-0.00103	0.00000	-0.00183	2.98953
A12	0.94046	-0.00167	-0.06088	0.00000	-0.05778	0.88268
A13	2.83248	0.00041	0.03412	0.00000	0.03217	2.86465
A14	2.51024	0.00126	0.02676	0.00000	0.02561	2.53585
A15	0.94775	-0.00409	-0.03290	0.00000	-0.03207	0.91569
A16	2.75995	0.00175	0.01748	0.00000	0.01695	2.77690
A17	2.57549	0.00233	0.01542	0.00000	0.01512	2.59060
A18	3.19935	-0.00103	-0.00802	0.00000	-0.00786	3.19149
A19	3.05630	-0.00015	0.00050	0.00000	0.00027	3.05657
A20	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
A21	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D1	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D2	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D4	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D5	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D6	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159

D7	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D8	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D9	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D10	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D11	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D12	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D13	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D14	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D15	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D16	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D17	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

Item	Value	Threshold	Converged?
Maximum Force	0.038973	0.000450	NO
RMS Force	0.007704	0.000300	NO
Maximum Displacement	0.202543	0.001800	NO
RMS Displacement	0.067302	0.001200	NO

Predicted change in Energy=-5.483977D-03
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.326972	2.891353	0.000000
2	1	0	1.811876	1.896921	0.000000
3	1	0	0.240262	2.638746	0.000000
4	6	0	-0.163311	-0.509876	0.000000
5	1	0	0.287224	-1.522031	0.000000
6	1	0	-1.276590	-0.625057	0.000000
7	6	0	-1.885820	-3.714139	0.000000
8	1	0	-1.365591	-4.720486	0.000000
9	1	0	-3.019768	-3.708368	0.000000
10	8	0	1.803227	3.973061	0.000000
11	8	0	0.429553	0.535271	0.000000
12	8	0	-1.276863	-2.723395	0.000000

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	H	1.106357	0.000000			
3	H	1.115683	1.737894	0.000000		
4	C	3.713395	3.113525	3.174381	0.000000	
5	H	4.534207	3.743501	4.161042	1.107898	0.000000
6	H	4.375348	3.987355	3.599062	1.119222	1.802797
7	C	7.345376	6.719892	6.699207	3.637903	3.086658
8	H	8.074031	7.340734	7.532401	4.378894	3.600265
9	H	7.902560	7.400274	7.135380	4.288320	3.964374
10	O	1.181910	2.076158	2.055056	4.895304	5.700378
11	O	2.521206	1.940337	2.111975	1.201591	2.062220
12	O	6.189132	5.557665	5.572632	2.477835	1.972218

		6	7	8	9	10
6	H	0.000000				
7	C	3.148586	0.000000			
8	H	4.096396	1.132860	0.000000		
9	H	3.541959	1.133962	1.939248	0.000000	
10	O	5.534253	8.526553	9.253062	9.070040	0.000000
11	O	2.063319	4.839260	5.553875	5.468664	3.702077
12	O	2.098339	1.162928	1.999061	2.001971	7.370853

		11	12
11	O	0.000000	
12	O	3.678419	0.000000

Stoichiometry C3H6O3
Framework group CS[SG(C3H6O3)]
Deg. of freedom 21
Full point group CS NOp 2
Largest Abelian subgroup CS NOp 2
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.393463	-3.152323	0.000000

```
  2        1           0     -1.156058   -2.350778    0.000000
  3        1           0      0.566209   -2.583308    0.000000
  4        6           0      0.000000    0.540169    0.000000
  5        1           0     -0.735184    1.368989    0.000000
  6        1           0      1.026506    0.986199    0.000000
  7        6           0      0.674332    4.115027    0.000000
  8        1           0     -0.125537    4.917262    0.000000
  9        1           0      1.757070    4.451996    0.000000
 10        8           0     -0.520784   -4.327355    0.000000
 11        8           0     -0.249527   -0.635228    0.000000
 12        8           0      0.393033    2.986633    0.000000
---------------------------------------------------------------------
Rotational constants (GHZ):     86.9600508      0.5950569      0.5910127
Isotopes: C-12,H-1,H-1,C-12,H-1,H-1,C-12,H-1,H-1,O-16,O-16,O-16
Standard basis: CBSB7 (5D, 7F)
There are   108 symmetry adapted basis functions of A'  symmetry.
There are    36 symmetry adapted basis functions of A"  symmetry.
Crude estimate of integral set expansion from redundant integrals=1.000.
Integral buffers will be    262144 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
  144 basis functions     240 primitive gaussians
   24 alpha electrons      24 beta electrons
     nuclear repulsion energy       192.4819154646 Hartrees.
One-electron integrals computed using PRISM.
NBasis=   144 RedAO= T  NBF=   108    36
NBsUse=   144 1.00D-04 NBFU=   108    36
Initial guess read from the read-write file:
Initial guess orbital symmetries:
     Occupied  (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A') (A") (A') (A") (A')
               (A") (A') (A') (A')
     Virtual   (A") (A") (A") (A') (A') (A') (A') (A') (A') (A')
               (A') (A') (A') (A") (A') (A') (A') (A") (A') (A")
               (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
               (A') (A") (A") (A") (A') (A') (A') (A") (A") (A')
               (A') (A") (A") (A') (A") (A") (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A') (A') (A") (A') (A')
               (A") (A") (A') (A") (A') (A") (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A') (A') (A') (A') (A")
               (A") (A') (A") (A') (A") (A") (A') (A') (A") (A')
               (A") (A") (A') (A") (A') (A') (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A") (A") (A") (A') (A')
               (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
Requested convergence on RMS density matrix=1.00D-08 within  64 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Integral accuracy reduced to 1.0D-05 until final iterations.
Initial convergence to 1.0D-05 achieved.  Increase integral accuracy.
SCF Done:  E(RB+HF-LYP) =  -343.588223518     A.U. after   11 cycles
          Convg  =    0.6718D-08           -V/T =  2.0020
          S**2   =   0.0000
***** Axes restored to original set *****
---------------------------------------------------------------------
Center     Atomic                 Forces (Hartrees/Bohr)
Number     Number           X              Y              Z
---------------------------------------------------------------------
  1        6        -0.023811097   -0.034022531    0.000000000
  2        1         0.021720571    0.012705193    0.000000000
  3        1        -0.002518306    0.017814783    0.000000000
  4        6        -0.006877879   -0.003897518    0.000000000
  5        1         0.012278747    0.012161699    0.000000000
  6        1         0.007340186    0.013840618    0.000000000
  7        6        -0.041091582   -0.067703173    0.000000000
  8        1        -0.009874576    0.007565846    0.000000000
  9        1         0.011710091   -0.004921203    0.000000000
 10        8         0.015493425    0.027250056    0.000000000
 11        8        -0.009369178   -0.020636689    0.000000000
 12        8         0.024999599    0.039842918    0.000000000
---------------------------------------------------------------------
Cartesian Forces:  Max     0.067703173 RMS     0.019425829

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Internal  Forces:  Max     0.075982091 RMS     0.012387557
```

Search for a local minimum.
Step number 6 out of a maximum of 63
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Update second derivatives using information from points 5 6
Eigenvalues --- 0.00230 0.01097 0.01345 0.01550 0.01975
Eigenvalues --- 0.03461 0.03565 0.03565 0.06161 0.06457
Eigenvalues --- 0.07750 0.09186 0.09357 0.13114 0.14731
Eigenvalues --- 0.16000 0.16032 0.18978 0.18979 0.19081
Eigenvalues --- 0.19115 0.33580 0.33843 0.36816 0.36861
Eigenvalues --- 0.37074 0.37230 0.79844 0.80209 0.94796
Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
Eigenvalues --- 1000.000001000.000001000.00000
RFO step: Lambda=-1.91030487D-02.
Quartic linear search produced a step of 0.26156.
Iteration 1 RMS(Cart)= 0.08254930 RMS(Int)= 0.00046461
Iteration 2 RMS(Cart)= 0.00028686 RMS(Int)= 0.00035356
Iteration 3 RMS(Cart)= 0.00000010 RMS(Int)= 0.00035356

Variable	Old X	-DE/DX (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.09071	0.00240	0.00316	0.00929	0.01215	2.10286
R2	2.10834	-0.00054	0.00423	0.00270	0.00660	2.11493
R3	2.23349	0.03118	-0.00803	0.03132	0.02329	2.25677
R4	4.76439	0.00224	0.06609	0.09094	0.15680	4.92119
R5	3.66671	0.01590	0.04916	0.14957	0.19902	3.86573
R6	3.99105	0.01103	0.03269	0.14029	0.17330	4.16435
R7	2.09362	-0.00187	0.00380	-0.00116	0.00217	2.09580
R8	2.11502	-0.00640	0.00502	-0.01148	-0.00693	2.10809
R9	2.27068	0.00345	-0.00597	-0.00096	-0.00692	2.26376
R10	4.68243	0.00695	0.04159	0.12907	0.17062	4.85304
R11	3.72695	0.01326	0.02817	0.15223	0.18065	3.90760
R12	3.96529	0.01002	0.02089	0.13823	0.15942	4.12470
R13	2.14080	-0.01126	0.00660	-0.02299	-0.01639	2.12441
R14	2.14288	-0.01173	0.00672	-0.02412	-0.01740	2.12548
R15	2.19762	0.07598	-0.01003	0.08466	0.07463	2.27225
A1	1.79610	0.01167	-0.01721	0.06345	0.04570	1.84179
A2	2.27316	-0.00873	0.01020	-0.04184	-0.03133	2.24183
A3	2.21393	-0.00294	0.00701	-0.02161	-0.01437	2.19957
A4	3.09078	-0.00135	0.00538	-0.00661	-0.00131	3.08947
A5	1.88649	0.00472	-0.01157	0.02788	0.01580	1.90230
A6	2.20681	-0.00271	0.00613	-0.01484	-0.00845	2.19836
A7	2.18988	-0.00201	0.00544	-0.01305	-0.00736	2.18253
A8	2.05300	-0.00725	-0.00219	-0.04272	-0.04492	2.00808
A9	2.11336	0.00409	0.00083	0.02375	0.02458	2.13794
A10	2.11683	0.00316	0.00136	0.01898	0.02033	2.13716
A11	2.98953	-0.00037	-0.00048	-0.00120	-0.00168	2.98785
A12	0.88268	0.00164	-0.01511	-0.00877	-0.02282	0.85986
A13	2.86465	-0.00134	0.00841	0.00272	0.01060	2.87525
A14	2.53585	-0.00030	0.00670	0.00606	0.01222	2.54807
A15	0.91569	-0.00318	-0.00839	-0.02999	-0.03695	0.87873
A16	2.77690	0.00121	0.00443	0.01354	0.01726	2.79415
A17	2.59060	0.00198	0.00395	0.01645	0.01969	2.61030
A18	3.19149	-0.00052	-0.00206	-0.00271	-0.00476	3.18672
A19	3.05657	-0.00033	0.00007	-0.00049	-0.00043	3.05614
A20	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
A21	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D1	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D2	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D4	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D5	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D6	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D7	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D8	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D9	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D10	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D11	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D12	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D13	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D14	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D15	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D16	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159

D17 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

Item	Value	Threshold	Converged?
Maximum Force	0.075982	0.000450	NO
RMS Force	0.012388	0.000300	NO
Maximum Displacement	0.230517	0.001800	NO
RMS Displacement	0.082549	0.001200	NO

Predicted change in Energy=-8.086475D-03
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.358918	2.970780	0.000000
2	1	0	1.879869	1.987470	0.000000
3	1	0	0.265799	2.730696	0.000000
4	6	0	-0.148740	-0.509080	0.000000
5	1	0	0.312624	-1.517609	0.000000
6	1	0	-1.258989	-0.617720	0.000000
7	6	0	-1.942751	-3.822082	0.000000
8	1	0	-1.454633	-4.834771	0.000000
9	1	0	-3.067426	-3.835420	0.000000
10	8	0	1.837763	4.064810	0.000000
11	8	0	0.440436	0.533946	0.000000
12	8	0	-1.309648	-2.799830	0.000000

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	H	1.112785	0.000000			
3	H	1.119174	1.776966	0.000000		
4	C	3.792422	3.216833	3.266189	0.000000	
5	H	4.608728	3.839510	4.248563	1.109048	0.000000
6	H	4.441934	4.079148	3.679249	1.115552	1.811013
7	C	7.552748	6.954374	6.914954	3.767553	3.224486
8	H	8.297150	7.593541	7.758619	4.518512	3.758558
9	H	8.118921	7.640796	7.363712	4.425298	4.098412
10	O	1.194234	2.077767	2.061779	4.986649	5.787008
11	O	2.604184	2.045654	2.203681	1.197928	2.055532
12	O	6.357766	5.752500	5.750543	2.568120	2.067814

		6	7	8	9	10
6	H	0.000000				
7	C	3.276502	0.000000			
8	H	4.221586	1.124187	0.000000		
9	H	3.691074	1.124754	1.897315	0.000000	
10	O	5.613908	8.746163	9.489068	9.299167	0.000000
11	O	2.052896	4.965336	5.693365	5.603253	3.797305
12	O	2.182698	1.202422	2.040099	2.040154	7.551787

		11	12
11	O	0.000000	
12	O	3.765216	0.000000

Stoichiometry C3H6O3
Framework group CS[SG(C3H6O3)]
Deg. of freedom 21
Full point group CS NOp 2
Largest Abelian subgroup CS NOp 2
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.472813	-3.229457	0.000000
2	1	0	-1.248290	-2.431382	0.000000
3	1	0	0.509332	-2.692856	0.000000
4	6	0	0.000000	0.533376	0.000000
5	1	0	-0.725337	1.372347	0.000000
6	1	0	1.035401	0.948589	0.000000
7	6	0	0.794436	4.216218	0.000000
8	1	0	0.042250	5.051690	0.000000
9	1	0	1.870374	4.543982	0.000000
10	8	0	-0.626119	-4.413810	0.000000
11	8	0	-0.273506	-0.632911	0.000000

```
 12        8           0      0.472942    3.057572    0.000000
---------------------------------------------------------------------
Rotational constants (GHZ):     85.0700163      0.5654052      0.5616721
Isotopes: C-12,H-1,H-1,C-12,H-1,H-1,C-12,H-1,H-1,O-16,O-16,O-16
Standard basis: CBSB7 (5D, 7F)
There are   108 symmetry adapted basis functions of A'  symmetry.
There are    36 symmetry adapted basis functions of A"  symmetry.
Crude estimate of integral set expansion from redundant integrals=1.000.
Integral buffers will be    262144 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
  144 basis functions      240 primitive gaussians
   24 alpha electrons       24 beta electrons
     nuclear repulsion energy       188.7441478696 Hartrees.
One-electron integrals computed using PRISM.
NBasis=   144 RedAO= T  NBF=   108    36
NBsUse=   144 1.00D-04 NBFU=   108    36
Initial guess read from the read-write file:
Initial guess orbital symmetries:
     Occupied  (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A') (A") (A') (A') (A")
               (A") (A') (A') (A')
     Virtual   (A") (A") (A") (A') (A') (A') (A') (A') (A') (A')
               (A') (A') (A') (A") (A') (A') (A") (A') (A') (A")
               (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
               (A') (A") (A") (A') (A") (A') (A') (A") (A') (A")
               (A') (A") (A") (A') (A") (A") (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A') (A') (A") (A') (A')
               (A') (A") (A") (A") (A") (A") (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A') (A') (A') (A') (A")
               (A") (A') (A") (A') (A") (A") (A') (A') (A") (A')
               (A") (A") (A') (A") (A') (A') (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A") (A") (A") (A') (A')
               (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
Requested convergence on RMS density matrix=1.00D-08 within  64 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Integral accuracy reduced to 1.0D-05 until final iterations.
Initial convergence to 1.0D-05 achieved.  Increase integral accuracy.
SCF Done:  E(RB+HF-LYP) =  -343.601616100     A.U. after   11 cycles
          Convg  =    0.5735D-08           -V/T =  2.0028
          S**2   =   0.0000
***** Axes restored to original set *****
---------------------------------------------------------------------
Center     Atomic                 Forces (Hartrees/Bohr)
Number     Number           X           Y           Z
---------------------------------------------------------------------
  1        6        -0.013945672  -0.018528957   0.000000000
  2        1         0.013776708   0.013127141   0.000000000
  3        1         0.001822380   0.014163352   0.000000000
  4        6        -0.009505495  -0.011634816   0.000000000
  5        1         0.009485731   0.009632146   0.000000000
  6        1         0.004867056   0.010788067   0.000000000
  7        6        -0.005773527  -0.009247380   0.000000000
  8        1        -0.002978848   0.008817003   0.000000000
  9        1         0.009422472   0.001229659   0.000000000
 10        8         0.005610343   0.007255845   0.000000000
 11        8        -0.002661029  -0.008133054   0.000000000
 12        8        -0.010120119  -0.017469006   0.000000000
---------------------------------------------------------------------
Cartesian Forces:  Max     0.018528957 RMS     0.008355115

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Internal  Forces:  Max     0.011383348 RMS     0.004122278
Search for a local minimum.
Step number   7 out of a maximum of  63
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Update second derivatives using information from points  6  7
Trust test= 1.66D+00 RLast= 4.45D-01 DXMaxT set to 6.00D-01
   Eigenvalues ---    0.00230   0.01117   0.01351   0.01554   0.01959
   Eigenvalues ---    0.02299   0.03565   0.03565   0.06137   0.06392
   Eigenvalues ---    0.07703   0.08889   0.09185   0.12622   0.13465
   Eigenvalues ---    0.16000   0.16472   0.18979   0.18981   0.19047
   Eigenvalues ---    0.19114   0.33310   0.34114   0.35772   0.36859
```

```
   Eigenvalues ---    0.36898   0.37230   0.80166   0.80729   1.14504
   Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
   Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
   Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
   Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
   Eigenvalues --- 1000.000001000.000001000.00000
RFO step:  Lambda=-1.14625779D-02.
Quartic linear search produced a step of  0.98902.
Iteration  1 RMS(Cart)=  0.07933081 RMS(Int)=  0.03827321
Iteration  2 RMS(Cart)=  0.04248405 RMS(Int)=  0.00102148
Iteration  3 RMS(Cart)=  0.00012394 RMS(Int)=  0.00101282
Iteration  4 RMS(Cart)=  0.00000008 RMS(Int)=  0.00101282
Variable      Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                        (Linear)    (Quad)   (Total)
   R1       2.10286  -0.00180   0.01201  -0.00793   0.00347   2.10632
   R2       2.11493  -0.00359   0.00652  -0.01175  -0.00600   2.10893
   R3       2.25677   0.00890   0.02303  -0.00497   0.01806   2.27484
   R4       4.92119  -0.00013   0.15508   0.11130   0.26580   5.18699
   R5       3.86573   0.01138   0.19683   0.17083   0.36835   4.23407
   R6       4.16435   0.00801   0.17140   0.15593   0.32802   4.49237
   R7       2.09580  -0.00197   0.00215  -0.00234  -0.00159   2.09421
   R8       2.10809  -0.00431  -0.00686  -0.00578  -0.01408   2.09401
   R9       2.26376   0.00913  -0.00685   0.01350   0.00666   2.27041
  R10       4.85304   0.00340   0.16874   0.11770   0.28622   5.13926
  R11       3.90760   0.00947   0.17867   0.15243   0.33184   4.23944
  R12       4.12470   0.00730   0.15767   0.14089   0.29945   4.42415
  R13       2.12441  -0.00924  -0.01621  -0.02049  -0.03670   2.08771
  R14       2.12548  -0.00944  -0.01721  -0.02067  -0.03788   2.08760
  R15       2.27225  -0.00103   0.07381  -0.05501   0.01881   2.29106
   A1       1.84179   0.00911   0.04520   0.05890   0.10293   1.94472
   A2       2.24183  -0.00654  -0.03099  -0.03601  -0.06634   2.17549
   A3       2.19957  -0.00257  -0.01421  -0.02288  -0.03659   2.16297
   A4       3.08947  -0.00107  -0.00129  -0.00271  -0.00417   3.08531
   A5       1.90230   0.00468   0.01563   0.03836   0.05246   1.95476
   A6       2.19836  -0.00283  -0.00835  -0.02168  -0.02927   2.16909
   A7       2.18253  -0.00186  -0.00728  -0.01668  -0.02319   2.15934
   A8       2.00808   0.00160  -0.04442   0.03315  -0.01127   1.99681
   A9       2.13794  -0.00083   0.02431  -0.01837   0.00595   2.14389
  A10       2.13716  -0.00077   0.02011  -0.01479   0.00532   2.14248
  A11       2.98785  -0.00015  -0.00166  -0.00148  -0.00273   2.98513
  A12       0.85986  -0.00013  -0.02257  -0.02069  -0.04081   0.81905
  A13       2.87525  -0.00031   0.01048   0.00978   0.01924   2.89449
  A14       2.54807   0.00044   0.01209   0.01092   0.02157   2.56964
  A15       0.87873  -0.00177  -0.03655  -0.02309  -0.05504   0.82369
  A16       2.79415   0.00062   0.01707   0.01045   0.02528   2.81944
  A17       2.61030   0.00115   0.01948   0.01264   0.02976   2.64006
  A18       3.18672  -0.00008  -0.00471  -0.00044  -0.00516   3.18156
  A19       3.05614  -0.00014  -0.00042  -0.00005  -0.00035   3.05579
  A20       3.14159   0.00000   0.00000   0.00000   0.00000   3.14159
  A21       3.14159   0.00000   0.00000   0.00000   0.00000   3.14159
   D1       3.14159   0.00000   0.00000   0.00000   0.00000   3.14159
   D2       3.14159   0.00000   0.00000   0.00000   0.00000   3.14159
   D3       0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
   D4       3.14159   0.00000   0.00000   0.00000   0.00000   3.14159
   D5       0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
   D6       3.14159   0.00000   0.00000   0.00000   0.00000   3.14159
   D7       0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
   D8       3.14159   0.00000   0.00000   0.00000   0.00000   3.14159
   D9       0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
  D10       3.14159   0.00000   0.00000   0.00000   0.00000   3.14159
  D11       0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
  D12       3.14159   0.00000   0.00000   0.00000   0.00000   3.14159
  D13       0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
  D14       0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
  D15       3.14159   0.00000   0.00000   0.00000   0.00000   3.14159
  D16       3.14159   0.00000   0.00000   0.00000   0.00000   3.14159
  D17       0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
     Item               Value     Threshold  Converged?
Maximum Force            0.011383     0.000450     NO
RMS     Force            0.004122     0.000300     NO
Maximum Displacement     0.315043     0.001800     NO
RMS     Displacement     0.121179     0.001200     NO
Predicted change in Energy=-8.525362D-03
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
```

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.406086	3.093210	0.000000
2	1	0	1.991509	2.144709	0.000000
3	1	0	0.307929	2.894456	0.000000
4	6	0	-0.142710	-0.525333	0.000000
5	1	0	0.348481	-1.518739	0.000000
6	1	0	-1.247678	-0.608625	0.000000
7	6	0	-2.025555	-3.973652	0.000000
8	1	0	-1.556420	-4.973861	0.000000
9	1	0	-3.130178	-3.987520	0.000000
10	8	0	1.889378	4.195727	0.000000
11	8	0	0.447274	0.521282	0.000000
12	8	0	-1.382448	-2.945904	0.000000

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	H	1.114618	0.000000			
3	H	1.115998	1.842977	0.000000		
4	C	3.936067	3.418189	3.449353	0.000000	
5	H	4.731659	4.015021	4.413382	1.108208	0.000000
6	H	4.554783	4.251256	3.832948	1.108102	1.837398
7	C	7.855997	7.319231	7.253692	3.928868	3.415061
8	H	8.593840	7.953731	8.086174	4.667760	3.945443
9	H	8.409187	7.989738	7.692995	4.572932	4.265671
10	O	1.203793	2.053560	2.047996	5.139824	5.918572
11	O	2.744837	2.240575	2.377261	1.201451	2.042412
12	O	6.651828	6.107203	6.080065	2.719580	2.243416

		6	7	8	9	10
6	H	0.000000				
7	C	3.453765	0.000000			
8	H	4.376141	1.104766	0.000000		
9	H	3.867911	1.104710	1.857306	0.000000	
10	O	5.737850	9.058999	9.795656	9.600077	0.000000
11	O	2.037045	5.130235	5.849050	5.755646	3.947304
12	O	2.341161	1.212374	2.035406	2.034582	7.855428

		11	12
11	O	0.000000	
12	O	3.920365	0.000000

Stoichiometry C3H6O3
Framework group CS[SG(C3H6O3)]
Deg. of freedom 21
Full point group CS NOp 2
Largest Abelian subgroup CS NOp 2
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.566458	-3.358287	0.000000
2	1	0	-1.376051	-2.592172	0.000000
3	1	0	0.443692	-2.883892	0.000000
4	6	0	0.000000	0.536806	0.000000
5	1	0	-0.730073	1.370543	0.000000
6	1	0	1.046414	0.901371	0.000000
7	6	0	0.933041	4.353275	0.000000
8	1	0	0.222533	5.199258	0.000000
9	1	0	1.996971	4.650662	0.000000
10	8	0	-0.750062	-4.547996	0.000000
11	8	0	-0.301082	-0.626308	0.000000
12	8	0	0.575771	3.194738	0.000000

Rotational constants (GHZ): 81.4836231 0.5239072 0.5205603
Isotopes: C-12,H-1,H-1,C-12,H-1,H-1,C-12,H-1,H-1,O-16,O-16,O-16
Standard basis: CBSB7 (5D, 7F)
There are 108 symmetry adapted basis functions of A' symmetry.
There are 36 symmetry adapted basis functions of A" symmetry.
Crude estimate of integral set expansion from redundant integrals=1.000.

Integral buffers will be 262144 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
144 basis functions 240 primitive gaussians
24 alpha electrons 24 beta electrons
nuclear repulsion energy 184.3155478681 Hartrees.
One-electron integrals computed using PRISM.
NBasis= 144 RedAO= T NBF= 108 36
NBsUse= 144 1.00D-04 NBFU= 108 36
Initial guess read from the read-write file:
Initial guess orbital symmetries:
Occupied (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
(A') (A') (A') (A') (A') (A') (A') (A") (A') (A")
(A") (A') (A') (A')
Virtual (A") (A") (A") (A') (A') (A') (A') (A') (A') (A')
(A') (A') (A') (A") (A') (A') (A') (A") (A') (A")
(A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
(A') (A") (A") (A') (A") (A') (A') (A") (A') (A')
(A") (A") (A") (A') (A") (A") (A') (A') (A') (A')
(A') (A') (A') (A') (A') (A') (A') (A') (A') (A")
(A') (A") (A") (A") (A") (A") (A') (A') (A') (A')
(A') (A') (A') (A') (A') (A') (A') (A') (A') (A")
(A") (A') (A") (A') (A") (A') (A") (A') (A") (A')
(A") (A') (A") (A") (A') (A') (A') (A') (A') (A')
(A') (A') (A') (A') (A') (A") (A") (A") (A') (A')
(A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
Requested convergence on RMS density matrix=1.00D-08 within 64 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Integral accuracy reduced to 1.0D-05 until final iterations.
Initial convergence to 1.0D-05 achieved. Increase integral accuracy.
SCF Done: E(RB+HF-LYP) = -343.612300034 A.U. after 11 cycles
Convg = 0.6838D-08 -V/T = 2.0031
S**2 = 0.0000
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.001433272	-0.002380276	0.000000000
2	1	0.002063856	0.008306354	0.000000000
3	1	0.004019442	0.005352035	0.000000000
4	6	-0.002933355	-0.005783129	0.000000000
5	1	0.004052470	0.005321753	0.000000000
6	1	0.001212780	0.004790348	0.000000000
7	6	0.006641847	0.010576574	0.000000000
8	1	0.003397611	0.000196142	0.000000000
9	1	-0.001408466	0.003007195	0.000000000
10	8	-0.001267766	-0.003823703	0.000000000
11	8	-0.001301040	-0.004092444	0.000000000
12	8	-0.013044107	-0.021470849	0.000000000

Cartesian Forces: Max 0.021470849 RMS 0.005480745

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Internal Forces: Max 0.016259741 RMS 0.002915186
Search for a local minimum.
Step number 8 out of a maximum of 63
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Update second derivatives using information from points 7 8
Trust test= 1.25D+00 RLast= 7.92D-01 DXMaxT set to 8.49D-01
Eigenvalues --- 0.00230 0.01137 0.01273 0.01358 0.01560
Eigenvalues --- 0.01944 0.03565 0.03565 0.06072 0.06360
Eigenvalues --- 0.07673 0.08808 0.08908 0.12528 0.13546
Eigenvalues --- 0.16000 0.16526 0.18979 0.18983 0.19054
Eigenvalues --- 0.19118 0.33435 0.34518 0.36923 0.36936
Eigenvalues --- 0.37230 0.37291 0.80240 0.80840 1.17373
Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
Eigenvalues --- 1000.000001000.000001000.00000
RFO step: Lambda=-2.77041219D-03.
Quartic linear search produced a step of 0.91582.

Iteration 1 RMS(Cart)= 0.07457355 RMS(Int)= 0.05133102
Iteration 2 RMS(Cart)= 0.05860455 RMS(Int)= 0.00155024
Iteration 3 RMS(Cart)= 0.00014722 RMS(Int)= 0.00154431
Iteration 4 RMS(Cart)= 0.00000012 RMS(Int)= 0.00154431

Variable	Old X	-DE/DX (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.10632	-0.00427	0.00317	-0.01327	-0.01145	2.09488
R2	2.10893	-0.00392	-0.00550	-0.00819	-0.01517	2.09376
R3	2.27484	-0.00401	0.01654	-0.01540	0.00114	2.27598
R4	5.18699	0.00065	0.24342	0.08942	0.33223	5.51922
R5	4.23407	0.00455	0.33734	0.07022	0.40849	4.64257
R6	4.49237	0.00312	0.30041	0.05694	0.35839	4.85076
R7	2.09421	-0.00175	-0.00145	-0.00154	-0.00479	2.08942
R8	2.09401	-0.00088	-0.01289	0.00755	-0.00719	2.08682
R9	2.27041	0.00395	0.00610	-0.00270	0.00340	2.27381
R10	5.13926	0.00153	0.26212	0.06084	0.32254	5.46180
R11	4.23944	0.00443	0.30391	0.06000	0.36489	4.60433
R12	4.42415	0.00336	0.27425	0.05365	0.32903	4.75318
R13	2.08771	0.00127	-0.03361	0.02963	-0.00398	2.08373
R14	2.08760	0.00137	-0.03469	0.03054	-0.00415	2.08345
R15	2.29106	-0.01626	0.01722	-0.02290	-0.00568	2.28538
A1	1.94472	0.00238	0.09427	-0.01991	0.07260	2.01733
A2	2.17549	-0.00155	-0.06075	0.01493	-0.04489	2.13060
A3	2.16297	-0.00084	-0.03351	0.00498	-0.02771	2.13526
A4	3.08531	-0.00014	-0.00382	0.00737	0.00346	3.08877
A5	1.95476	0.00218	0.04805	0.00138	0.04746	2.00222
A6	2.16909	-0.00144	-0.02681	-0.00186	-0.02768	2.14140
A7	2.15934	-0.00073	-0.02124	0.00047	-0.01978	2.13956
A8	1.99681	0.00430	-0.01032	0.02994	0.01962	2.01643
A9	2.14389	-0.00229	0.00544	-0.01603	-0.01059	2.13330
A10	2.14248	-0.00201	0.00488	-0.01390	-0.00903	2.13346
A11	2.98513	0.00016	-0.00250	0.00013	-0.00196	2.98316
A12	0.81905	-0.00173	-0.03737	-0.02282	-0.05507	0.76398
A13	2.89449	0.00070	0.01762	0.01215	0.02741	2.92190
A14	2.56964	0.00103	0.01975	0.01067	0.02766	2.59730
A15	0.82369	-0.00068	-0.05041	-0.00973	-0.05376	0.76993
A16	2.81944	0.00026	0.02316	0.00498	0.02501	2.84445
A17	2.64006	0.00042	0.02725	0.00475	0.02875	2.66881
A18	3.18156	0.00015	-0.00473	-0.00001	-0.00474	3.17682
A19	3.05579	0.00014	-0.00032	0.00086	0.00067	3.05646
A20	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
A21	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D1	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D2	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D4	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D5	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D6	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D7	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D8	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D9	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D10	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D11	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D12	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D13	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D14	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D15	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D16	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D17	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

Item	Value	Threshold	Converged?
Maximum Force	0.016260	0.000450	NO
RMS Force	0.002915	0.000300	NO
Maximum Displacement	0.348641	0.001800	NO
RMS Displacement	0.132588	0.001200	NO

Predicted change in Energy=-5.267189D-03
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.473248	3.248713	0.000000
2	1	0	2.102094	2.335772	0.000000

```
  3        1           0      0.378844    3.075859    0.000000
  4        6           0     -0.132899   -0.537945    0.000000
  5        1           0      0.384305   -1.515192    0.000000
  6        1           0     -1.235507   -0.599031    0.000000
  7        6           0     -2.108721   -4.126508    0.000000
  8        1           0     -1.634096   -5.121793    0.000000
  9        1           0     -3.211234   -4.125780    0.000000
 10        8           0      1.950919    4.354335    0.000000
 11        8           0      0.458088    0.510171    0.000000
 12        8           0     -1.462921   -3.104003    0.000000
---------------------------------------------------------------------
            Distance matrix (angstroms):
                  1        2        3        4        5
  1  C    0.000000
  2  H    1.108561   0.000000
  3  H    1.107970   1.875452   0.000000
  4  C    4.113208   3.640528   3.649857   0.000000
  5  H    4.886776   4.216719   4.591054   1.105672   0.000000
  6  H    4.705580   4.444395   4.013844   1.104299   1.860952
  7  C    8.199048   7.713108   7.619847   4.096542   3.610284
  8  H    8.928659   8.341127   8.441174   4.823407   4.132979
  9  H    8.736562   8.365591   8.046879   4.727442   4.443317
 10  O    1.204396   2.024215   2.026307   5.317584   6.074999
 11  O    2.920644   2.456741   2.566911   1.203251   2.026706
 12  O    6.998435   6.503883   6.448472   2.890262   2.436507
                  6        7        8        9       10
  6  H    0.000000
  7  C    3.633951   0.000000
  8  H    4.540292   1.102660   0.000000
  9  H    4.042457   1.102513   1.865316   0.000000
 10  O    5.889748   9.402413  10.131600   9.927747   0.000000
 11  O    2.024498   5.299745   6.008015   5.912357   4.123850
 12  O    2.515274   1.209369   2.025037   2.025000   8.202506
                 11       12
 11  O    0.000000
 12  O    4.092986   0.000000
Stoichiometry    C3H6O3
Framework group  CS[SG(C3H6O3)]
Deg. of freedom   21
Full point group                 CS     NOp   2
Largest Abelian subgroup         CS     NOp   2
Largest concise Abelian subgroup C1     NOp   1
                    Standard orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic           Coordinates (Angstroms)
Number     Number     Type             X         Y         Z
---------------------------------------------------------------------
  1        6           0     -0.676375   -3.511665    0.000000
  2        1           0     -1.501227   -2.771038    0.000000
  3        1           0      0.347290   -3.087746    0.000000
  4        6           0      0.000000    0.545551    0.000000
  5        1           0     -0.731336    1.374802    0.000000
  6        1           0      1.057773    0.862717    0.000000
  7        6           0      1.082118    4.496586    0.000000
  8        1           0      0.387964    5.353330    0.000000
  9        1           0      2.154249    4.753629    0.000000
 10        8           0     -0.882332   -4.698320    0.000000
 11        8           0     -0.329576   -0.611684    0.000000
 12        8           0      0.693261    3.351438    0.000000
---------------------------------------------------------------------
Rotational constants (GHZ):     77.3881096      0.4823029      0.4793157
Isotopes: C-12,H-1,H-1,C-12,H-1,H-1,C-12,H-1,H-1,O-16,O-16,O-16
Standard basis: CBSB7 (5D, 7F)
There are   108 symmetry adapted basis functions of A'  symmetry.
There are    36 symmetry adapted basis functions of A"  symmetry.
Crude estimate of integral set expansion from redundant integrals=1.000.
Integral buffers will be    262144 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
  144 basis functions      240 primitive gaussians
   24 alpha electrons       24 beta electrons
     nuclear repulsion energy       180.1568030343 Hartrees.
One-electron integrals computed using PRISM.
NBasis=   144 RedAO= T  NBF=   108    36
```

```
NBsUse=   144 1.00D-04 NBFU=   108    36
Initial guess read from the read-write file:
Initial guess orbital symmetries:
     Occupied  (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A') (A") (A') (A")
               (A") (A') (A') (A')
     Virtual   (A") (A") (A") (A') (A') (A') (A') (A') (A') (A')
               (A') (A') (A') (A") (A') (A') (A') (A") (A') (A')
               (A") (A') (A') (A') (A') (A') (A') (A') (A') (A')
               (A') (A") (A") (A") (A') (A') (A') (A') (A") (A')
               (A") (A") (A") (A') (A") (A") (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
               (A") (A") (A") (A") (A") (A") (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A') (A') (A') (A') (A")
               (A') (A") (A') (A") (A") (A') (A") (A') (A") (A')
               (A") (A') (A") (A") (A') (A') (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A") (A") (A") (A') (A')
               (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
Requested convergence on RMS density matrix=1.00D-08 within  64 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Integral accuracy reduced to 1.0D-05 until final iterations.
Initial convergence to 1.0D-05 achieved.  Increase integral accuracy.
SCF Done:  E(RB+HF-LYP) =  -343.616608884     A.U. after   11 cycles
          Convg  =    0.1397D-08           -V/T =  2.0031
          S**2   =   0.0000
***** Axes restored to original set *****
-------------------------------------------------------------------
Center     Atomic                   Forces (Hartrees/Bohr)
Number     Number           X              Y              Z
-------------------------------------------------------------------
   1        6         0.003848765    0.004002956    0.000000000
   2        1        -0.002525447    0.000624074    0.000000000
   3        1         0.001071936   -0.001240892    0.000000000
   4        6         0.001233412   -0.000334416    0.000000000
   5        1         0.000255662    0.000936610    0.000000000
   6        1        -0.000745647    0.000284842    0.000000000
   7        6         0.006576952    0.010118956    0.000000000
   8        1         0.002141953   -0.001862944    0.000000000
   9        1        -0.002728447    0.001109775    0.000000000
  10        8        -0.001288879   -0.001082847    0.000000000
  11        8        -0.000285627   -0.000551241    0.000000000
  12        8        -0.007554635   -0.012004871    0.000000000
-------------------------------------------------------------------
Cartesian Forces:  Max     0.012004871 RMS     0.003375971

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Internal  Forces:  Max     0.011117568 RMS     0.001789763
Search for a local minimum.
Step number   9 out of a maximum of  63
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Update second derivatives using information from points  8  9
Trust test= 8.18D-01 RLast= 8.79D-01 DXMaxT set to 1.00D+00
    Eigenvalues ---    0.00230   0.00640   0.01151   0.01354   0.01565
    Eigenvalues ---    0.01933   0.03565   0.03565   0.05914   0.06348
    Eigenvalues ---    0.07663   0.08344   0.09066   0.13011   0.13885
    Eigenvalues ---    0.16000   0.16513   0.18980   0.18985   0.19066
    Eigenvalues ---    0.19117   0.33846   0.34848   0.36972   0.36981
    Eigenvalues ---    0.37181   0.37230   0.80278   0.80783   1.15247
    Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
    Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
    Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
    Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
    Eigenvalues --- 1000.000001000.000001000.00000
RFO step:  Lambda=-6.65146568D-04.
Quartic linear search produced a step of  0.52146.
Iteration  1 RMS(Cart)=  0.07766099 RMS(Int)=  0.00814108
Iteration  2 RMS(Cart)=  0.00956962 RMS(Int)=  0.00081153
Iteration  3 RMS(Cart)=  0.00002427 RMS(Int)=  0.00081122
Iteration  4 RMS(Cart)=  0.00000001 RMS(Int)=  0.00081122
Variable      Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                        (Linear)    (Quad)   (Total)
   R1       2.09488  -0.00161  -0.00597   0.00130  -0.00552   2.08936
   R2       2.09376  -0.00057  -0.00791   0.00475  -0.00403   2.08973
```

R3	2.27598	-0.00151	0.00059	-0.00025	0.00034	2.27632
R4	5.51922	0.00222	0.17324	0.06265	0.23562	5.75483
R5	4.64257	0.00018	0.21301	0.03106	0.24455	4.88712
R6	4.85076	-0.00008	0.18688	0.01848	0.20594	5.05670
R7	2.08942	-0.00043	-0.00250	0.00228	-0.00099	2.08842
R8	2.08682	0.00088	-0.00375	0.00644	0.00191	2.08873
R9	2.27381	0.00193	0.00177	0.00037	0.00214	2.27595
R10	5.46180	0.00144	0.16819	0.04124	0.20921	5.67102
R11	4.60433	0.00103	0.19028	0.02575	0.21646	4.82079
R12	4.75318	0.00067	0.17157	0.02103	0.19309	4.94627
R13	2.08373	0.00260	-0.00208	0.01068	0.00861	2.09233
R14	2.08345	0.00273	-0.00217	0.01106	0.00889	2.09234
R15	2.28538	-0.01112	-0.00296	-0.00915	-0.01211	2.27327
A1	2.01733	-0.00217	0.03786	-0.03195	0.00493	2.02225
A2	2.13060	0.00166	-0.02341	0.02108	-0.00184	2.12875
A3	2.13526	0.00050	-0.01445	0.01086	-0.00309	2.13218
A4	3.08877	0.00056	0.00180	0.00790	0.00972	3.09848
A5	2.00222	-0.00046	0.02475	-0.01375	0.01013	2.01235
A6	2.14140	0.00023	-0.01444	0.00770	-0.00630	2.13510
A7	2.13956	0.00022	-0.01031	0.00605	-0.00382	2.13574
A8	2.01643	0.00156	0.01023	-0.00091	0.00932	2.02576
A9	2.13330	-0.00080	-0.00552	0.00067	-0.00485	2.12844
A10	2.13346	-0.00075	-0.00471	0.00024	-0.00447	2.12899
A11	2.98316	0.00019	-0.00102	0.00005	-0.00095	2.98222
A12	0.76398	-0.00098	-0.02872	-0.01100	-0.03646	0.72753
A13	2.92190	0.00044	0.01429	0.00605	0.01873	2.94063
A14	2.59730	0.00054	0.01442	0.00495	0.01773	2.61503
A15	0.76993	-0.00017	-0.02804	-0.00589	-0.03103	0.73889
A16	2.84445	0.00007	0.01304	0.00294	0.01454	2.85899
A17	2.66881	0.00011	0.01499	0.00295	0.01650	2.68530
A18	3.17682	-0.00004	-0.00247	-0.00180	-0.00427	3.17255
A19	3.05646	0.00016	0.00035	0.00051	0.00086	3.05732
A20	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
A21	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D1	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D2	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D4	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D5	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D6	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D7	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D8	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D9	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D10	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D11	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D12	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D13	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D14	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D15	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D16	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D17	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

Item	Value	Threshold	Converged?
Maximum Force	0.011118	0.000450	NO
RMS Force	0.001790	0.000300	NO
Maximum Displacement	0.221524	0.001800	NO
RMS Displacement	0.085439	0.001200	NO

Predicted change in Energy=-1.069543D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.525498	3.362979	0.000000
2	1	0	2.164240	2.460510	0.000000
3	1	0	0.434582	3.181926	0.000000
4	6	0	-0.120913	-0.542964	0.000000
5	1	0	0.402419	-1.516346	0.000000
6	1	0	-1.224743	-0.600145	0.000000
7	6	0	-2.158225	-4.216763	0.000000
8	1	0	-1.679964	-5.215358	0.000000
9	1	0	-3.265407	-4.207565	0.000000
10	8	0	1.991159	4.473911	0.000000

```
 11        8           0      0.470382    0.506278    0.000000
 12        8           0     -1.512622   -3.201720    0.000000
---------------------------------------------------------------------
             Distance matrix (angstroms):
                  1        2        3        4        5
  1  C    0.000000
  2  H    1.105641   0.000000
  3  H    1.105839   1.874076   0.000000
  4  C    4.238757   3.773961   3.766083   0.000000
  5  H    5.006907   4.349643   4.698382   1.105147   0.000000
  6  H    4.823917   4.566488   4.130063   1.105310   1.867373
  7  C    8.427473   7.954224   7.839850   4.200885   3.721445
  8  H    9.157667   8.584687   8.659428   4.925638   4.244881
  9  H    8.959125   8.599087   8.264049   4.828783   4.549243
 10  O    1.204578   2.020826   2.022908   5.443333   6.197359
 11  O    3.045327   2.586152   2.675888   1.204383   2.023765
 12  O    7.233633   6.751308   6.674020   3.000972   2.551052
                  6        7        8        9       10
  6  H    0.000000
  7  C    3.735146   0.000000
  8  H    4.637609   1.107216   0.000000
  9  H    4.144610   1.107220   1.878637   0.000000
 10  O    6.007334   9.630430  10.361422  10.148867   0.000000
 11  O    2.024258   5.405246   6.112373   6.014685   4.249103
 12  O    2.617454   1.202961   2.020580   2.020886   8.437522
                 11       12
 11  O    0.000000
 12  O    4.204943   0.000000
Stoichiometry    C3H6O3
Framework group  CS[SG(C3H6O3)]
Deg. of freedom   21
Full point group                 CS     NOp   2
Largest Abelian subgroup         CS     NOp   2
Largest concise Abelian subgroup C1     NOp   1
                    Standard orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic           Coordinates (Angstroms)
Number     Number      Type             X         Y         Z
---------------------------------------------------------------------
   1         6           0      -0.771515   -3.613146    0.000000
   2         1           0      -1.588746   -2.868448    0.000000
   3         1           0       0.255297   -3.202614    0.000000
   4         6           0       0.000000    0.554806    0.000000
   5         1           0      -0.719690    1.393493    0.000000
   6         1           0       1.065960    0.847108    0.000000
   7         6           0       1.203069    4.579736    0.000000
   8         1           0       0.522003    5.452706    0.000000
   9         1           0       2.286521    4.807918    0.000000
  10         8           0      -0.988398   -4.798039    0.000000
  11         8           0      -0.352815   -0.596740    0.000000
  12         8           0       0.789880    3.449962    0.000000
---------------------------------------------------------------------
Rotational constants (GHZ):     74.7041676      0.4571169      0.4543368
Isotopes: C-12,H-1,H-1,C-12,H-1,H-1,C-12,H-1,H-1,O-16,O-16,O-16
Standard basis: CBSB7 (5D, 7F)
There are   108 symmetry adapted basis functions of A'  symmetry.
There are    36 symmetry adapted basis functions of A"  symmetry.
Crude estimate of integral set expansion from redundant integrals=1.000.
Integral buffers will be    262144 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
  144 basis functions      240 primitive gaussians
   24 alpha electrons       24 beta electrons
     nuclear repulsion energy       177.6351689044 Hartrees.
One-electron integrals computed using PRISM.
NBasis=   144 RedAO= T  NBF=   108    36
NBsUse=   144 1.00D-04 NBFU=   108    36
Initial guess read from the read-write file:
Initial guess orbital symmetries:
     Occupied  (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A') (A') (A") (A') (A")
               (A") (A') (A') (A')
     Virtual   (A") (A") (A") (A') (A') (A') (A') (A') (A') (A')
               (A') (A') (A') (A') (A") (A') (A') (A") (A') (A")
```

(A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
(A') (A") (A") (A") (A') (A') (A') (A') (A") (A')
(A") (A") (A") (A') (A") (A") (A') (A') (A') (A')
(A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
(A") (A") (A") (A") (A") (A") (A') (A') (A') (A')
(A') (A') (A') (A') (A') (A') (A') (A') (A') (A")
(A') (A") (A') (A") (A") (A') (A") (A') (A") (A')
(A") (A') (A") (A") (A') (A') (A') (A') (A') (A')
(A') (A') (A') (A') (A') (A") (A") (A") (A') (A')
(A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
Requested convergence on RMS density matrix=1.00D-08 within 64 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Integral accuracy reduced to 1.0D-05 until final iterations.
Initial convergence to 1.0D-05 achieved. Increase integral accuracy.
SCF Done: E(RB+HF-LYP) = -343.617488411 A.U. after 10 cycles
Convg = 0.5070D-08 -V/T = 2.0031
S**2 = 0.0000
***** Axes restored to original set *****

Center Atomic Forces (Hartrees/Bohr)
Number Number X Y Z
---
1 6 0.003425158 0.005377409 0.000000000
2 1 -0.001581766 -0.001497265 0.000000000
3 1 -0.000325936 -0.001912947 0.000000000
4 6 0.001674262 0.001885099 0.000000000
5 1 -0.000425243 -0.000238400 0.000000000
6 1 -0.000292605 -0.000532844 0.000000000
7 6 0.001107982 0.001574457 0.000000000
8 1 -0.000063739 -0.000363779 0.000000000
9 1 -0.000326616 -0.000207830 0.000000000
10 8 -0.001191658 -0.001446164 0.000000000
11 8 -0.000679176 -0.000692361 0.000000000
12 8 -0.001320663 -0.001945376 0.000000000

Cartesian Forces: Max 0.005377409 RMS 0.001395380

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Internal Forces: Max 0.001975095 RMS 0.000573463
Search for a local minimum.
Step number 10 out of a maximum of 63
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Update second derivatives using information from points 9 10
Trust test= 8.22D-01 RLast= 5.38D-01 DXMaxT set to 1.00D+00
Eigenvalues --- 0.00230 0.00329 0.01162 0.01345 0.01569
Eigenvalues --- 0.01923 0.03565 0.03565 0.05790 0.06335
Eigenvalues --- 0.07652 0.08024 0.08993 0.12820 0.13552
Eigenvalues --- 0.16000 0.16691 0.18980 0.18986 0.19046
Eigenvalues --- 0.19121 0.33977 0.35052 0.36988 0.36990
Eigenvalues --- 0.37230 0.37785 0.80290 0.81609 1.17965
Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
Eigenvalues --- 1000.000001000.000001000.00000
RFO step: Lambda=-1.23738942D-04.
Quartic linear search produced a step of 0.45665.
Iteration 1 RMS(Cart)= 0.04556419 RMS(Int)= 0.00025105
Iteration 2 RMS(Cart)= 0.00008341 RMS(Int)= 0.00024305
Iteration 3 RMS(Cart)= 0.00000001 RMS(Int)= 0.00024305
Variable Old X -DE/DX Delta X Delta X Delta X New X
(Linear) (Quad) (Total)
R1 2.08936 0.00024 -0.00252 0.00313 0.00036 2.08971
R2 2.08973 0.00062 -0.00184 0.00344 0.00134 2.09108
R3 2.27632 -0.00179 0.00016 -0.00318 -0.00303 2.27330
R4 5.75483 0.00163 0.10759 0.02360 0.13106 5.88589
R5 4.88712 -0.00054 0.11167 0.00977 0.12161 5.00872
R6 5.05670 -0.00061 0.09404 0.00260 0.09683 5.15353
R7 2.08842 0.00007 -0.00045 0.00125 0.00058 2.08900
R8 2.08873 0.00036 0.00087 0.00110 0.00176 2.09049
R9 2.27595 -0.00032 0.00098 -0.00168 -0.00070 2.27525
R10 5.67102 0.00097 0.09554 0.01654 0.11200 5.78302
R11 4.82079 0.00013 0.09885 0.00896 0.10793 4.92872

R12	4.94627	0.00000	0.08818	0.00658	0.09490	5.04117
R13	2.09233	0.00030	0.00393	-0.00090	0.00303	2.09536
R14	2.09234	0.00032	0.00406	-0.00092	0.00314	2.09548
R15	2.27327	-0.00123	-0.00553	0.00157	-0.00396	2.26931
A1	2.02225	-0.00198	0.00225	-0.01485	-0.01294	2.00932
A2	2.12875	0.00140	-0.00084	0.00902	0.00834	2.13709
A3	2.13218	0.00058	-0.00141	0.00584	0.00460	2.13678
A4	3.09848	0.00041	0.00444	0.00331	0.00776	3.10624
A5	2.01235	-0.00078	0.00462	-0.00724	-0.00287	2.00948
A6	2.13510	0.00050	-0.00288	0.00431	0.00156	2.13666
A7	2.13574	0.00028	-0.00175	0.00293	0.00131	2.13705
A8	2.02576	-0.00030	0.00426	-0.00576	-0.00150	2.02426
A9	2.12844	0.00015	-0.00222	0.00290	0.00069	2.12913
A10	2.12899	0.00014	-0.00204	0.00286	0.00081	2.12980
A11	2.98222	0.00009	-0.00043	0.00004	-0.00043	2.98178
A12	0.72753	-0.00023	-0.01665	-0.00323	-0.01887	0.70865
A13	2.94063	0.00008	0.00855	0.00162	0.00965	2.95028
A14	2.61503	0.00015	0.00810	0.00161	0.00923	2.62426
A15	0.73889	-0.00012	-0.01417	-0.00256	-0.01592	0.72298
A16	2.85899	0.00002	0.00664	0.00105	0.00728	2.86627
A17	2.68530	0.00010	0.00753	0.00151	0.00864	2.69394
A18	3.17255	-0.00013	-0.00195	-0.00126	-0.00321	3.16934
A19	3.05732	0.00007	0.00039	0.00022	0.00060	3.05792
A20	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
A21	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D1	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D2	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D4	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D5	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D6	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D7	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D8	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D9	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D10	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D11	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D12	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D13	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D14	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D15	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D16	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D17	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

Item	Value	Threshold	Converged?
Maximum Force	0.001975	0.000450	NO
RMS Force	0.000573	0.000300	NO
Maximum Displacement	0.119878	0.001800	NO
RMS Displacement	0.045578	0.001200	NO

Predicted change in Energy=-1.765799D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.554179	3.424907	0.000000
2	1	0	2.193392	2.522541	0.000000
3	1	0	0.465074	3.229194	0.000000
4	6	0	-0.112660	-0.547144	0.000000
5	1	0	0.409830	-1.521326	0.000000
6	1	0	-1.217312	-0.606422	0.000000
7	6	0	-2.185648	-4.266561	0.000000
8	1	0	-1.709447	-5.267915	0.000000
9	1	0	-3.294479	-4.255962	0.000000
10	8	0	2.009510	4.538383	0.000000
11	8	0	0.477883	0.502095	0.000000
12	8	0	-1.539077	-3.254617	0.000000

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	H	1.105829	0.000000			
3	H	1.106550	1.867201	0.000000		
4	C	4.307615	3.839380	3.820276	0.000000	

```
  5  H    5.076885   4.419723   4.750842   1.105453   0.000000
  6  H    4.892114   4.628532   4.188361   1.106241   1.866719
  7  C    8.552484   8.078854   7.950639   4.258091   3.777938
  8  H    9.285280   8.713401   8.770941   4.983514   4.304447
  9  H    9.083239   8.721514   8.376263   4.886645   4.604360
 10  O    1.202977   2.024211   2.024662   5.510553   6.267300
 11  O    3.114682   2.650503   2.727129   1.204012   2.024566
 12  O    7.360997   6.877999   6.786489   3.060241   2.608167
                6          7          8          9         10
  6  H    0.000000
  7  C    3.786065   0.000000
  8  H    4.687400   1.108819   0.000000
  9  H    4.199257   1.108881   1.880525   0.000000
 10  O    6.073005   9.753275  10.487808  10.269994   0.000000
 11  O    2.025462   5.462095   6.170692   6.072052   4.317116
 12  O    2.667671   1.200868   2.020494   2.020922   8.562903
                11         12
 11  O    0.000000
 12  O    4.263920   0.000000
Stoichiometry    C3H6O3
Framework group  CS[SG(C3H6O3)]
Deg. of freedom   21
Full point group                 CS     NOp   2
Largest Abelian subgroup         CS     NOp   2
Largest concise Abelian subgroup C1     NOp   1
                     Standard orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic           Coordinates (Angstroms)
Number     Number      Type             X           Y           Z
---------------------------------------------------------------------
   1         6          0       -0.838053   -3.665708    0.000000
   2         1          0       -1.644950   -2.909549    0.000000
   3         1          0        0.189837   -3.255958    0.000000
   4         6          0        0.000000    0.559598    0.000000
   5         1          0       -0.706911    1.409483    0.000000
   6         1          0        1.070432    0.838786    0.000000
   7         6          0        1.286551    4.618677    0.000000
   8         1          0        0.619554    5.504450    0.000000
   9         1          0        2.375064    4.830239    0.000000
  10         8          0       -1.061294   -4.847789    0.000000
  11         8          0       -0.368575   -0.586612    0.000000
  12         8          0        0.855617    3.497794    0.000000
---------------------------------------------------------------------
Rotational constants (GHZ):     73.2352178      0.4443457      0.4416659
Isotopes: C-12,H-1,H-1,C-12,H-1,H-1,C-12,H-1,H-1,O-16,O-16,O-16
Standard basis: CBSB7 (5D, 7F)
There are   108 symmetry adapted basis functions of A'  symmetry.
There are    36 symmetry adapted basis functions of A"  symmetry.
Crude estimate of integral set expansion from redundant integrals=1.000.
Integral buffers will be    262144 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
  144 basis functions      240 primitive gaussians
   24 alpha electrons       24 beta electrons
     nuclear repulsion energy       176.3574567243 Hartrees.
One-electron integrals computed using PRISM.
NBasis=   144 RedAO= T  NBF=   108    36
NBsUse=   144 1.00D-04 NBFU=   108    36
Initial guess read from the read-write file:
Initial guess orbital symmetries:
     Occupied  (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A') (A") (A') (A")
               (A") (A') (A') (A')
     Virtual   (A") (A") (A") (A') (A') (A') (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A") (A') (A") (A') (A")
               (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
               (A') (A") (A") (A") (A') (A') (A') (A') (A") (A')
               (A") (A") (A") (A') (A") (A") (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
               (A") (A") (A") (A") (A") (A") (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A') (A') (A') (A') (A")
               (A') (A') (A") (A") (A") (A') (A") (A') (A") (A')
               (A") (A") (A') (A") (A') (A') (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A") (A") (A") (A') (A')
```

(A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
Requested convergence on RMS density matrix=1.00D-08 within 64 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Integral accuracy reduced to 1.0D-05 until final iterations.
Initial convergence to 1.0D-05 achieved. Increase integral accuracy.
SCF Done: E(RB+HF-LYP) = -343.617655506 A.U. after 10 cycles
Convg = 0.4305D-08 -V/T = 2.0031
S**2 = 0.0000
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.001111478	0.002120331	0.000000000
2	1	-0.000305481	-0.001097698	0.000000000
3	1	-0.000502532	-0.000982143	0.000000000
4	6	0.000723830	0.001122111	0.000000000
5	1	-0.000173950	-0.000256174	0.000000000
6	1	-0.000003755	-0.000316471	0.000000000
7	6	-0.000934940	-0.001573100	0.000000000
8	1	-0.000403191	0.000281216	0.000000000
9	1	0.000439725	-0.000234556	0.000000000
10	8	-0.000246380	-0.000129846	0.000000000
11	8	-0.000350461	-0.000134535	0.000000000
12	8	0.000645657	0.001200865	0.000000000

Cartesian Forces: Max 0.002120331 RMS 0.000669617

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Internal Forces: Max 0.001770105 RMS 0.000351951
Search for a local minimum.
Step number 11 out of a maximum of 63
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Update second derivatives using information from points 10 11
Trust test= 9.46D-01 RLast= 2.75D-01 DXMaxT set to 1.00D+00
Eigenvalues --- 0.00225 0.00230 0.01168 0.01335 0.01571
Eigenvalues --- 0.01918 0.03565 0.03565 0.05723 0.06334
Eigenvalues --- 0.07595 0.07854 0.08732 0.11916 0.13437
Eigenvalues --- 0.16000 0.16648 0.18976 0.18987 0.19033
Eigenvalues --- 0.19122 0.33997 0.35079 0.36990 0.36994
Eigenvalues --- 0.37230 0.38240 0.80264 0.81315 1.22136
Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
Eigenvalues --- 1000.000001000.000001000.00000
RFO step: Lambda=-1.68985349D-05.
Quartic linear search produced a step of 0.31197.
Iteration 1 RMS(Cart)= 0.01396321 RMS(Int)= 0.00003339
Iteration 2 RMS(Cart)= 0.00001199 RMS(Int)= 0.00003200
Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00003200

Variable	Old X	-DE/DX (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.08971	0.00062	0.00011	0.00193	0.00201	2.09172
R2	2.09108	0.00058	0.00042	0.00159	0.00198	2.09306
R3	2.27330	-0.00021	-0.00094	-0.00008	-0.00102	2.27228
R4	5.88589	0.00060	0.04089	-0.00096	0.03990	5.92580
R5	5.00872	-0.00029	0.03794	-0.00390	0.03407	5.04279
R6	5.15353	-0.00040	0.03021	-0.00636	0.02387	5.17740
R7	2.08900	0.00016	0.00018	0.00057	0.00072	2.08972
R8	2.09049	0.00003	0.00055	0.00001	0.00053	2.09102
R9	2.27525	-0.00034	-0.00022	-0.00036	-0.00057	2.27468
R10	5.78302	0.00043	0.03494	0.00002	0.03495	5.81796
R11	4.92872	0.00003	0.03367	-0.00183	0.03186	4.96058
R12	5.04117	-0.00007	0.02961	-0.00288	0.02675	5.06791
R13	2.09536	-0.00043	0.00094	-0.00156	-0.00061	2.09475
R14	2.09548	-0.00044	0.00098	-0.00161	-0.00063	2.09485
R15	2.26931	0.00177	-0.00123	0.00203	0.00079	2.27011
A1	2.00932	-0.00076	-0.00404	-0.00376	-0.00784	2.00148
A2	2.13709	0.00051	0.00260	0.00195	0.00457	2.14166
A3	2.13678	0.00026	0.00144	0.00181	0.00327	2.14005
A4	3.10624	0.00016	0.00242	0.00071	0.00313	3.10937
A5	2.00948	-0.00038	-0.00089	-0.00225	-0.00318	2.00630

A6	2.13666	0.00025	0.00049	0.00130	0.00180	2.13846
A7	2.13705	0.00013	0.00041	0.00095	0.00138	2.13843
A8	2.02426	-0.00033	-0.00047	-0.00130	-0.00177	2.02249
A9	2.12913	0.00018	0.00021	0.00072	0.00093	2.13006
A10	2.12980	0.00015	0.00025	0.00059	0.00084	2.13064
A11	2.98178	0.00004	-0.00013	0.00014	0.00000	2.98178
A12	0.70865	0.00008	-0.00589	0.00050	-0.00526	0.70339
A13	2.95028	-0.00008	0.00301	-0.00045	0.00249	2.95276
A14	2.62426	-0.00001	0.00288	-0.00005	0.00277	2.62703
A15	0.72298	-0.00005	-0.00497	-0.00007	-0.00493	0.71805
A16	2.86627	-0.00002	0.00227	-0.00018	0.00203	2.86830
A17	2.69394	0.00007	0.00270	0.00025	0.00289	2.69683
A18	3.16934	-0.00009	-0.00100	-0.00045	-0.00145	3.16789
A19	3.05792	0.00003	0.00019	0.00015	0.00033	3.05826
A20	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
A21	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D1	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D2	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D4	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D5	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D6	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D7	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D8	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D9	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D10	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D11	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D12	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D13	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D14	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D15	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D16	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D17	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

Item	Value	Threshold	Converged?
Maximum Force	0.001770	0.000450	NO
RMS Force	0.000352	0.000300	NO
Maximum Displacement	0.038831	0.001800	NO
RMS Displacement	0.013965	0.001200	NO

Predicted change in Energy=-1.924954D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.563101	3.443212	0.000000
2	1	0	2.202017	2.539335	0.000000
3	1	0	0.474329	3.239870	0.000000
4	6	0	-0.109159	-0.549112	0.000000
5	1	0	0.412173	-1.524346	0.000000
6	1	0	-1.213979	-0.610405	0.000000
7	6	0	-2.194480	-4.283325	0.000000
8	1	0	-1.720042	-5.285159	0.000000
9	1	0	-3.302977	-4.272895	0.000000
10	8	0	2.014258	4.557802	0.000000
11	8	0	0.480785	0.500117	0.000000
12	8	0	-1.546984	-3.271475	0.000000

Distance matrix (angstroms):

		1	2	3	4	5	6	7	8	9	10
1	C	0.000000									
2	H	1.106891	0.000000								
3	H	1.107597	1.864311	0.000000							
4	C	4.328406	3.857465	3.833645	0.000000						
5	H	5.099144	4.440388	4.764621	1.105834	0.000000					
6	H	4.913653	4.646492	4.204164	1.106519	1.865385					
7	C	8.591786	8.116519	7.982544	4.277022	3.795604					
8	H	9.325421	8.752442	8.802918	5.002508	4.323199					
9	H	9.122337	8.758507	8.408905	4.905817	4.621349					
10	O	1.202436	2.027181	2.026901	5.530775	6.289610					
11	O	3.135797	2.668530	2.739761	1.203708	2.025625					
12	O	7.399976	6.915238	6.817867	3.078733	2.625025					

```
  6  H    0.000000
  7  C    3.801543   0.000000
  8  H    4.702066   1.108495   0.000000
  9  H    4.216367   1.108547   1.878926   0.000000
 10  O    6.093593   9.791783  10.527529  10.307968   0.000000
 11  O    2.026199   5.480726   6.189753   6.090853   4.337782
 12  O    2.681825   1.201288   2.021107   2.021474   8.601164
           11         12
 11  O    0.000000
 12  O    4.282142   0.000000
Stoichiometry    C3H6O3
Framework group  CS[SG(C3H6O3)]
Deg. of freedom   21
Full point group                 CS      NOp   2
Largest Abelian subgroup         CS      NOp   2
Largest concise Abelian subgroup C1      NOp   1
                    Standard orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic           Coordinates (Angstroms)
Number     Number      Type             X         Y         Z
---------------------------------------------------------------------
  1         6           0      -0.864182   -3.680563    0.000000
  2         1           0      -1.666635   -2.918148    0.000000
  3         1           0       0.164282   -3.269426    0.000000
  4         6           0       0.000000    0.560698    0.000000
  5         1           0      -0.700986    1.415969    0.000000
  6         1           0       1.071823    0.835615    0.000000
  7         6           0       1.319542    4.629079    0.000000
  8         1           0       0.659385    5.519558    0.000000
  9         1           0       2.408916    4.834357    0.000000
 10         8           0      -1.090037   -4.861597    0.000000
 11         8           0      -0.374701   -0.583205    0.000000
 12         8           0       0.881120    3.510651    0.000000
---------------------------------------------------------------------
Rotational constants (GHZ):     72.7484524      0.4405031      0.4378519
Isotopes: C-12,H-1,H-1,C-12,H-1,H-1,C-12,H-1,H-1,O-16,O-16,O-16
Standard basis: CBSB7 (5D, 7F)
There are   108 symmetry adapted basis functions of A'  symmetry.
There are    36 symmetry adapted basis functions of A"  symmetry.
Crude estimate of integral set expansion from redundant integrals=1.000.
Integral buffers will be    262144 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
  144 basis functions      240 primitive gaussians
   24 alpha electrons       24 beta electrons
     nuclear repulsion energy       175.9553793821 Hartrees.
One-electron integrals computed using PRISM.
NBasis=   144 RedAO= T  NBF=   108    36
NBsUse=   144 1.00D-04 NBFU=   108    36
Initial guess read from the read-write file:
Initial guess orbital symmetries:
     Occupied  (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A') (A') (A') (A") (A")
               (A") (A') (A') (A')
     Virtual   (A") (A") (A") (A') (A') (A') (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A") (A') (A") (A') (A")
               (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
               (A') (A") (A") (A") (A') (A') (A') (A') (A") (A')
               (A") (A") (A") (A') (A") (A") (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
               (A") (A") (A") (A") (A") (A") (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A') (A') (A') (A') (A")
               (A') (A') (A") (A") (A") (A') (A") (A') (A") (A')
               (A") (A") (A') (A") (A') (A') (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A") (A") (A") (A') (A')
               (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
Requested convergence on RMS density matrix=1.00D-08 within  64 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Integral accuracy reduced to 1.0D-05 until final iterations.
Initial convergence to 1.0D-05 achieved.  Increase integral accuracy.
SCF Done:  E(RB+HF-LYP) =  -343.617676284     A.U. after   10 cycles
          Convg  =    0.1303D-08           -V/T =  2.0031
          S**2   =    0.0000
***** Axes restored to original set *****
```

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000167362	0.000350523	0.000000000
2	1	0.000055694	-0.000334324	0.000000000
3	1	-0.000193361	-0.000301844	0.000000000
4	6	0.000246140	0.000364256	0.000000000
5	1	0.000035012	-0.000042224	0.000000000
6	1	0.000034340	-0.000067327	0.000000000
7	6	-0.000571425	-0.000979576	0.000000000
8	1	-0.000147889	0.000191347	0.000000000
9	1	0.000244994	-0.000050634	0.000000000
10	8	-0.000037861	0.000048391	0.000000000
11	8	-0.000146593	0.000146960	0.000000000
12	8	0.000313587	0.000674451	0.000000000

Cartesian Forces: Max 0.000979576 RMS 0.000268922

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Internal Forces: Max 0.000962342 RMS 0.000157728
Search for a local minimum.
Step number 12 out of a maximum of 63
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Update second derivatives using information from points 10 11 12
Trust test= 1.08D+00 RLast= 8.06D-02 DXMaxT set to 1.00D+00
Eigenvalues --- 0.00214 0.00230 0.01170 0.01332 0.01572
Eigenvalues --- 0.01917 0.03565 0.03565 0.05705 0.06326
Eigenvalues --- 0.07071 0.07802 0.08777 0.11502 0.13514
Eigenvalues --- 0.16000 0.16658 0.18953 0.18988 0.19018
Eigenvalues --- 0.19121 0.33897 0.34971 0.36971 0.36993
Eigenvalues --- 0.37230 0.37500 0.80187 0.80858 1.18793
Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
Eigenvalues --- 1000.000001000.000001000.00000
RFO step: Lambda=-2.06590675D-06.
Quartic linear search produced a step of 0.21179.
Iteration 1 RMS(Cart)= 0.00144522 RMS(Int)= 0.00000133
Iteration 2 RMS(Cart)= 0.00000058 RMS(Int)= 0.00000122

Variable	Old X	-DE/DX (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.09172	0.00026	0.00042	0.00046	0.00088	2.09261
R2	2.09306	0.00019	0.00042	0.00030	0.00072	2.09377
R3	2.27228	0.00003	-0.00022	0.00004	-0.00018	2.27210
R4	5.92580	0.00004	0.00845	-0.00576	0.00269	5.92849
R5	5.04279	-0.00006	0.00721	-0.00509	0.00213	5.04492
R6	5.17740	-0.00020	0.00506	-0.00621	-0.00116	5.17624
R7	2.08972	0.00007	0.00015	0.00013	0.00028	2.09000
R8	2.09102	-0.00002	0.00011	-0.00008	0.00003	2.09105
R9	2.27468	-0.00015	-0.00012	-0.00009	-0.00021	2.27446
R10	5.81796	0.00015	0.00740	-0.00301	0.00439	5.82235
R11	4.96058	0.00009	0.00675	-0.00280	0.00395	4.96453
R12	5.06791	-0.00002	0.00566	-0.00351	0.00215	5.07007
R13	2.09475	-0.00024	-0.00013	-0.00057	-0.00070	2.09406
R14	2.09485	-0.00025	-0.00013	-0.00058	-0.00072	2.09413
R15	2.27011	0.00096	0.00017	0.00072	0.00089	2.27100
A1	2.00148	-0.00011	-0.00166	-0.00015	-0.00182	1.99966
A2	2.14166	0.00008	0.00097	-0.00002	0.00095	2.14261
A3	2.14005	0.00003	0.00069	0.00017	0.00086	2.14091
A4	3.10937	0.00007	0.00066	0.00020	0.00086	3.11024
A5	2.00630	-0.00009	-0.00067	-0.00031	-0.00099	2.00531
A6	2.13846	0.00007	0.00038	0.00019	0.00058	2.13904
A7	2.13843	0.00002	0.00029	0.00012	0.00042	2.13884
A8	2.02249	-0.00007	-0.00038	0.00011	-0.00026	2.02222
A9	2.13006	0.00004	0.00020	-0.00005	0.00015	2.13021
A10	2.13064	0.00003	0.00018	-0.00006	0.00012	2.13075
A11	2.98178	0.00002	0.00000	0.00015	0.00015	2.98193
A12	0.70339	0.00007	-0.00111	0.00092	-0.00019	0.70320
A13	2.95276	-0.00007	0.00053	-0.00065	-0.00013	2.95264
A14	2.62703	0.00000	0.00059	-0.00026	0.00032	2.62735
A15	0.71805	-0.00002	-0.00104	0.00041	-0.00063	0.71742

A16	2.86830	-0.00003	0.00043	-0.00039	0.00004	2.86834
A17	2.69683	0.00005	0.00061	-0.00002	0.00059	2.69742
A18	3.16789	-0.00006	-0.00031	-0.00022	-0.00053	3.16736
A19	3.05826	0.00003	0.00007	0.00015	0.00022	3.05848
A20	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
A21	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D1	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D2	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D4	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D5	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D6	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D7	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D8	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D9	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D10	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D11	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D12	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D13	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D14	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D15	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D16	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D17	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

Item	Value	Threshold	Converged?
Maximum Force	0.000962	0.000450	NO
RMS Force	0.000158	0.000300	YES
Maximum Displacement	0.004231	0.001800	NO
RMS Displacement	0.001445	0.001200	NO

Predicted change in Energy=-1.701022D-06

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.563954	3.444214	0.000000
2	1	0	2.203155	2.539965	0.000000
3	1	0	0.475184	3.238808	0.000000
4	6	0	-0.108161	-0.549614	0.000000
5	1	0	0.412930	-1.525146	0.000000
6	1	0	-1.212958	-0.611651	0.000000
7	6	0	-2.195618	-4.285850	0.000000
8	1	0	-1.721538	-5.287446	0.000000
9	1	0	-3.303736	-4.275494	0.000000
10	8	0	2.013996	4.559154	0.000000
11	8	0	0.481458	0.499666	0.000000
12	8	0	-1.547814	-3.273636	0.000000

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	H	1.107359	0.000000			
3	H	1.107977	1.863938	0.000000		
4	C	4.329738	3.858456	3.833071	0.000000	
5	H	5.100921	4.441850	4.764360	1.105983	0.000000
6	H	4.915413	4.647850	4.204266	1.106537	1.864936
7	C	8.595829	8.120404	7.984589	4.279829	3.798159
8	H	9.329328	8.756232	8.804692	5.005001	4.325605
9	H	9.126243	8.762211	8.411003	4.908552	4.623638
10	O	1.202342	2.028029	2.027623	5.532003	6.291431
11	O	3.137222	2.669656	2.739149	1.203595	2.025971
12	O	7.403554	6.918651	6.819417	3.081055	2.627116

		6	7	8	9	10
6	H	0.000000				
7	C	3.803336	0.000000			
8	H	4.703373	1.108127	0.000000		
9	H	4.218424	1.108167	1.878137	0.000000	
10	O	6.095116	9.795659	10.531370	10.311609	0.000000
11	O	2.026344	5.483421	6.192242	6.093427	4.339137
12	O	2.682964	1.201760	2.021290	2.021629	8.604597

		11	12
11	O	0.000000	
12	O	4.284362	0.000000

Stoichiometry C3H6O3
Framework group CS[SG(C3H6O3)]
Deg. of freedom 21
Full point group CS NOp 2
Largest Abelian subgroup CS NOp 2
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.870613	-3.680903	0.000000
2	1	0	-1.672182	-2.916879	0.000000
3	1	0	0.158116	-3.269406	0.000000
4	6	0	0.000000	0.560402	0.000000
5	1	0	-0.699421	1.417145	0.000000
6	1	0	1.072100	0.834310	0.000000
7	6	0	1.327831	4.629039	0.000000
8	1	0	0.669513	5.520422	0.000000
9	1	0	2.417150	4.832553	0.000000
10	8	0	-1.097217	-4.861698	0.000000
11	8	0	-0.376223	-0.582881	0.000000
12	8	0	0.887368	3.510907	0.000000

Rotational constants (GHZ): 72.6549917 0.4401394 0.4374891
Isotopes: C-12,H-1,H-1,C-12,H-1,H-1,C-12,H-1,H-1,O-16,O-16,O-16
Standard basis: CBSB7 (5D, 7F)
There are 108 symmetry adapted basis functions of A' symmetry.
There are 36 symmetry adapted basis functions of A" symmetry.
Crude estimate of integral set expansion from redundant integrals=1.000.
Integral buffers will be 262144 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
144 basis functions 240 primitive gaussians
24 alpha electrons 24 beta electrons
nuclear repulsion energy 175.9114256164 Hartrees.
One-electron integrals computed using PRISM.
NBasis= 144 RedAO= T NBF= 108 36
NBsUse= 144 1.00D-04 NBFU= 108 36
Initial guess read from the read-write file:
Initial guess orbital symmetries:
Occupied (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
(A') (A') (A') (A') (A') (A') (A') (A') (A") (A")
(A") (A') (A') (A')
Virtual (A") (A") (A") (A') (A') (A') (A') (A') (A') (A')
(A') (A') (A') (A') (A') (A") (A') (A") (A') (A")
(A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
(A') (A") (A") (A") (A') (A') (A') (A') (A") (A')
(A") (A") (A") (A') (A") (A") (A') (A') (A') (A')
(A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
(A") (A") (A") (A") (A") (A") (A') (A') (A') (A')
(A') (A') (A') (A') (A') (A') (A') (A') (A') (A")
(A') (A') (A") (A") (A") (A') (A") (A') (A") (A')
(A") (A") (A') (A") (A') (A') (A') (A') (A') (A')
(A') (A') (A') (A') (A') (A") (A") (A") (A') (A')
(A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
Requested convergence on RMS density matrix=1.00D-08 within 64 cycles.
Requested convergence on MAX density matrix=1.00D-06.
SCF Done: E(RB+HF-LYP) = -343.617678510 A.U. after 8 cycles
Convg = 0.2277D-08 -V/T = 2.0031
S**2 = 0.0000
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000000383	-0.000107396	0.000000000
2	1	0.000048881	-0.000052296	0.000000000
3	1	-0.000032665	-0.000123761	0.000000000
4	6	0.000125100	0.000085666	0.000000000
5	1	0.000088553	0.000050533	0.000000000
6	1	0.000017090	0.000005967	0.000000000
7	6	-0.000107691	-0.000254682	0.000000000
8	1	-0.000016151	0.000049064	0.000000000

```
  9        1        0.000054236   0.000006019   0.000000000
 10        8       -0.000028340   0.000037867   0.000000000
 11        8       -0.000069377   0.000247512   0.000000000
 12        8       -0.000079253   0.000055507   0.000000000
---------------------------------------------------------------------
Cartesian Forces:  Max     0.000254682 RMS     0.000079326

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Internal  Forces:  Max     0.000205743 RMS     0.000047269
Search for a local minimum.
Step number  13 out of a maximum of  63
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Update second derivatives using information from points 10 11 12 13
Trust test= 1.31D+00 RLast= 8.02D-03 DXMaxT set to 1.00D+00
    Eigenvalues ---    0.00225   0.00230   0.01170   0.01332   0.01572
    Eigenvalues ---    0.01916   0.03565   0.03565   0.03905   0.05704
    Eigenvalues ---    0.06597   0.07796   0.09191   0.12639   0.13962
    Eigenvalues ---    0.16000   0.16766   0.18619   0.18989   0.19012
    Eigenvalues ---    0.19129   0.33937   0.35065   0.36980   0.36994
    Eigenvalues ---    0.37230   0.37348   0.80302   0.80907   1.15658
    Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
    Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
    Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
    Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
    Eigenvalues --- 1000.000001000.000001000.00000
RFO step:  Lambda=-1.00748422D-06.
Quartic linear search produced a step of  0.59345.
Iteration  1 RMS(Cart)=  0.00120711 RMS(Int)=  0.00000048
Iteration  2 RMS(Cart)=  0.00000051 RMS(Int)=  0.00000018
Variable      Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                        (Linear)    (Quad)   (Total)
    R1        2.09261   0.00006   0.00052   0.00002   0.00054   2.09315
    R2        2.09377   0.00003   0.00043  -0.00004   0.00039   2.09416
    R3        2.27210   0.00002  -0.00011   0.00004  -0.00006   2.27203
    R4        5.92849  -0.00009   0.00160  -0.00119   0.00041   5.92890
    R5        5.04492   0.00000   0.00126   0.00027   0.00153   5.04645
    R6        5.17624  -0.00014  -0.00069  -0.00210  -0.00279   5.17345
    R7        2.09000   0.00002   0.00017   0.00002   0.00018   2.09019
    R8        2.09105  -0.00001   0.00002  -0.00002   0.00000   2.09105
    R9        2.27446  -0.00004  -0.00013   0.00000  -0.00012   2.27434
   R10        5.82235   0.00008   0.00260   0.00162   0.00422   5.82657
   R11        4.96453   0.00012   0.00235   0.00239   0.00473   4.96926
   R12        5.07007   0.00001   0.00128   0.00083   0.00211   5.07218
   R13        2.09406  -0.00005  -0.00041  -0.00008  -0.00049   2.09357
   R14        2.09413  -0.00005  -0.00043  -0.00008  -0.00050   2.09363
   R15        2.27100   0.00021   0.00053   0.00006   0.00059   2.27159
    A1        1.99966   0.00002  -0.00108   0.00021  -0.00087   1.99879
    A2        2.14261   0.00001   0.00057  -0.00016   0.00040   2.14301
    A3        2.14091  -0.00003   0.00051  -0.00004   0.00047   2.14138
    A4        3.11024   0.00006   0.00051   0.00052   0.00104   3.11127
    A5        2.00531  -0.00001  -0.00059   0.00010  -0.00049   2.00481
    A6        2.13904   0.00002   0.00034  -0.00007   0.00027   2.13931
    A7        2.13884  -0.00001   0.00025  -0.00003   0.00022   2.13906
    A8        2.02222   0.00001  -0.00016   0.00018   0.00003   2.02225
    A9        2.13021   0.00000   0.00009  -0.00009   0.00000   2.13021
   A10        2.13075  -0.00001   0.00007  -0.00009  -0.00002   2.13073
   A11        2.98193   0.00002   0.00009   0.00017   0.00025   2.98218
   A12        0.70320   0.00003  -0.00011   0.00019   0.00008   0.70328
   A13        2.95264  -0.00005  -0.00008  -0.00032  -0.00040   2.95224
   A14        2.62735   0.00002   0.00019   0.00013   0.00032   2.62767
   A15        0.71742  -0.00001  -0.00037  -0.00021  -0.00058   0.71684
   A16        2.86834  -0.00003   0.00002  -0.00015  -0.00013   2.86821
   A17        2.69742   0.00004   0.00035   0.00036   0.00071   2.69813
   A18        3.16736  -0.00004  -0.00031  -0.00036  -0.00067   3.16668
   A19        3.05848   0.00003   0.00013   0.00022   0.00035   3.05883
   A20        3.14159   0.00000   0.00000   0.00000   0.00000   3.14159
   A21        3.14159   0.00000   0.00000   0.00000   0.00000   3.14159
    D1        3.14159   0.00000   0.00000   0.00000   0.00000   3.14159
    D2        3.14159   0.00000   0.00000   0.00000   0.00000   3.14159
    D3        0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
    D4        3.14159   0.00000   0.00000   0.00000   0.00000   3.14159
    D5        0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
    D6        3.14159   0.00000   0.00000   0.00000   0.00000   3.14159
```

D7	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D8	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D9	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D10	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D11	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D12	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D13	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D14	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D15	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D16	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D17	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

Item	Value	Threshold	Converged?
Maximum Force	0.000206	0.000450	YES
RMS Force	0.000047	0.000300	YES
Maximum Displacement	0.002760	0.001800	NO
RMS Displacement	0.001207	0.001200	NO

Predicted change in Energy=-8.982433D-07
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.564369	3.444927	0.000000
2	1	0	2.204394	2.540910	0.000000
3	1	0	0.475726	3.237742	0.000000
4	6	0	-0.107150	-0.549352	0.000000
5	1	0	0.414062	-1.524928	0.000000
6	1	0	-1.211912	-0.612015	0.000000
7	6	0	-2.196685	-4.287371	0.000000
8	1	0	-1.722692	-5.288722	0.000000
9	1	0	-3.304536	-4.277015	0.000000
10	8	0	2.013139	4.560343	0.000000
11	8	0	0.482072	0.500077	0.000000
12	8	0	-1.548735	-3.274878	0.000000

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	H	1.107646	0.000000			
3	H	1.108183	1.863832	0.000000		
4	C	4.329924	3.859139	3.831687	0.000000	
5	H	5.101242	4.442559	4.763070	1.106080	0.000000
6	H	4.915946	4.648880	4.203422	1.106538	1.864726
7	C	8.598486	8.123725	7.985556	4.282399	3.800932
8	H	9.331742	8.759289	8.805319	5.007156	4.328032
9	H	9.128781	8.765410	8.412013	4.911085	4.626225
10	O	1.202309	2.028470	2.028032	5.532144	6.291866
11	O	3.137437	2.670467	2.737673	1.203530	2.026147
12	O	7.405890	6.921660	6.820020	3.083287	2.629619

		6	7	8	9	10
6	H	0.000000				
7	C	3.804999	0.000000			
8	H	4.704517	1.107869	0.000000		
9	H	4.220344	1.107900	1.877706	0.000000	
10	O	6.095429	9.798197	10.533780	10.313902	0.000000
11	O	2.026409	5.485927	6.194448	6.095819	4.339347
12	O	2.684081	1.202073	2.021343	2.021662	8.606837

		11	12
11	O	0.000000	
12	O	4.286545	0.000000

Stoichiometry C3H6O3
Framework group CS[SG(C3H6O3)]
Deg. of freedom 21
Full point group CS NOp 2
Largest Abelian subgroup CS NOp 2
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.877762	-3.680161	0.000000

```
  2        1           0     -1.678686   -2.915046    0.000000
  3        1           0      0.151259   -3.268841    0.000000
  4        6           0      0.000000    0.559859    0.000000
  5        1           0     -0.697967    1.417912    0.000000
  6        1           0      1.072450    0.832398    0.000000
  7        6           0      1.337031    4.628187    0.000000
  8        1           0      0.680490    5.520559    0.000000
  9        1           0      2.426461    4.829641    0.000000
 10        8           0     -1.105205   -4.860762    0.000000
 11        8           0     -0.377913   -0.582798    0.000000
 12        8           0      0.894416    3.510568    0.000000
---------------------------------------------------------------------
Rotational constants (GHZ):     72.5433901      0.4399018      0.4372504
Isotopes: C-12,H-1,H-1,C-12,H-1,H-1,C-12,H-1,H-1,O-16,O-16,O-16
Standard basis: CBSB7 (5D, 7F)
There are   108 symmetry adapted basis functions of A'  symmetry.
There are    36 symmetry adapted basis functions of A"  symmetry.
Crude estimate of integral set expansion from redundant integrals=1.000.
Integral buffers will be    262144 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
  144 basis functions      240 primitive gaussians
   24 alpha electrons       24 beta electrons
     nuclear repulsion energy       175.8817518848 Hartrees.
One-electron integrals computed using PRISM.
NBasis=   144 RedAO= T  NBF=   108    36
NBsUse=   144 1.00D-04 NBFU=   108    36
Initial guess read from the read-write file:
Initial guess orbital symmetries:
     Occupied  (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A') (A') (A') (A") (A")
               (A") (A') (A') (A')
     Virtual   (A") (A") (A") (A') (A') (A') (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A") (A') (A") (A') (A")
               (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
               (A') (A") (A") (A") (A') (A') (A') (A') (A") (A')
               (A") (A") (A") (A') (A") (A") (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
               (A") (A") (A") (A") (A") (A") (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A') (A') (A') (A') (A")
               (A') (A') (A") (A") (A") (A') (A") (A') (A") (A')
               (A") (A") (A') (A") (A') (A') (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A") (A") (A") (A') (A')
               (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
Requested convergence on RMS density matrix=1.00D-08 within  64 cycles.
Requested convergence on MAX density matrix=1.00D-06.
SCF Done:  E(RB+HF-LYP) =  -343.617679680     A.U. after    8 cycles
          Convg  =    0.1295D-08           -V/T =  2.0031
          S**2   =   0.0000
***** Axes restored to original set *****
---------------------------------------------------------------------
Center     Atomic                 Forces (Hartrees/Bohr)
Number     Number           X              Y              Z
---------------------------------------------------------------------
  1        6        -0.000061687   -0.000333782    0.000000000
  2        1         0.000022186    0.000107539    0.000000000
  3        1         0.000063380   -0.000031749    0.000000000
  4        6         0.000062971   -0.000076475    0.000000000
  5        1         0.000110533    0.000102314    0.000000000
  6        1         0.000003530    0.000042159    0.000000000
  7        6         0.000213792    0.000248465    0.000000000
  8        1         0.000057512   -0.000059129    0.000000000
  9        1        -0.000079414    0.000025120    0.000000000
 10        8        -0.000037936    0.000011892    0.000000000
 11        8        -0.000025750    0.000302958    0.000000000
 12        8        -0.000329116   -0.000339313    0.000000000
---------------------------------------------------------------------
Cartesian Forces:  Max     0.000339313 RMS     0.000129663

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Internal  Forces:  Max     0.000283964 RMS     0.000059268
Search for a local minimum.
Step number  14 out of a maximum of  63
```

All quantities printed in internal units (Hartrees-Bohrs-Radians)
Update second derivatives using information from points 10 11 12 13 14

Trust test= 1.30D+00 RLast= 7.78D-03 DXMaxT set to 1.00D+00
Eigenvalues --- 0.00206 0.00230 0.01171 0.01332 0.01345
Eigenvalues --- 0.01573 0.01916 0.03565 0.03565 0.05704
Eigenvalues --- 0.06602 0.07791 0.09101 0.13034 0.13857
Eigenvalues --- 0.16001 0.16697 0.18053 0.18987 0.19015
Eigenvalues --- 0.19142 0.34051 0.35215 0.36987 0.36994
Eigenvalues --- 0.37230 0.43894 0.80324 0.82049 1.61215
Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
Eigenvalues --- 1000.000001000.000001000.00000
RFO step: Lambda=-3.17134207D-06.
Quartic linear search produced a step of 2.00000.
Iteration 1 RMS(Cart)= 0.00500644 RMS(Int)= 0.00000473
Iteration 2 RMS(Cart)= 0.00000532 RMS(Int)= 0.00000158
Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000158

Variable	Old X	-DE/DX (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.09315	-0.00007	0.00108	-0.00011	0.00098	2.09412
R2	2.09416	-0.00007	0.00078	-0.00013	0.00065	2.09481
R3	2.27203	0.00000	-0.00013	-0.00001	-0.00013	2.27190
R4	5.92890	-0.00015	0.00081	0.00401	0.00482	5.93371
R5	5.04645	0.00003	0.00306	0.00693	0.00999	5.05644
R6	5.17345	-0.00011	-0.00558	0.00101	-0.00457	5.16888
R7	2.09019	-0.00001	0.00037	0.00000	0.00036	2.09055
R8	2.09105	0.00000	0.00000	0.00000	0.00000	2.09106
R9	2.27434	0.00003	-0.00025	0.00002	-0.00023	2.27411
R10	5.82657	0.00004	0.00844	0.00878	0.01721	5.84378
R11	4.96926	0.00013	0.00946	0.01036	0.01982	4.98908
R12	5.07218	0.00002	0.00422	0.00669	0.01091	5.08308
R13	2.09357	0.00008	-0.00098	0.00013	-0.00085	2.09272
R14	2.09363	0.00008	-0.00101	0.00013	-0.00088	2.09275
R15	2.27159	-0.00028	0.00118	-0.00019	0.00100	2.27259
A1	1.99879	0.00008	-0.00174	0.00020	-0.00154	1.99725
A2	2.14301	-0.00002	0.00080	-0.00019	0.00061	2.14363
A3	2.14138	-0.00006	0.00094	-0.00001	0.00093	2.14231
A4	3.11127	0.00005	0.00207	0.00136	0.00343	3.11470
A5	2.00481	0.00003	-0.00098	0.00031	-0.00068	2.00414
A6	2.13931	-0.00001	0.00054	-0.00022	0.00032	2.13963
A7	2.13906	-0.00003	0.00044	-0.00009	0.00035	2.13942
A8	2.02225	0.00004	0.00005	0.00003	0.00008	2.02233
A9	2.13021	-0.00002	0.00000	-0.00002	-0.00003	2.13018
A10	2.13073	-0.00002	-0.00005	-0.00001	-0.00006	2.13067
A11	2.98218	0.00003	0.00051	0.00028	0.00079	2.98297
A12	0.70328	0.00000	0.00015	-0.00053	-0.00038	0.70290
A13	2.95224	-0.00003	-0.00079	-0.00015	-0.00094	2.95130
A14	2.62767	0.00003	0.00064	0.00067	0.00132	2.62899
A15	0.71684	0.00000	-0.00116	-0.00118	-0.00234	0.71451
A16	2.86821	-0.00003	-0.00026	0.00008	-0.00018	2.86803
A17	2.69813	0.00004	0.00142	0.00110	0.00251	2.70065
A18	3.16668	-0.00004	-0.00135	-0.00083	-0.00218	3.16451
A19	3.05883	0.00003	0.00070	0.00043	0.00113	3.05996
A20	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
A21	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D1	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D2	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D4	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D5	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D6	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D7	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D8	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D9	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D10	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D11	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D12	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D13	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D14	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D15	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D16	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159

```
 D17       0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
     Item               Value     Threshold  Converged?
Maximum Force            0.000284     0.000450     YES
RMS     Force            0.000059     0.000300     YES
Maximum Displacement     0.011788     0.001800     NO
RMS     Displacement     0.005007     0.001200     NO
Predicted change in Energy=-3.251491D-06
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

                         Input orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic           Coordinates (Angstroms)
Number     Number      Type             X           Y           Z
---------------------------------------------------------------------
    1          6           0        1.566276    3.449368    0.000000
    2          1           0        2.209416    2.546928    0.000000
    3          1           0        0.478273    3.237048    0.000000
    4          6           0       -0.104039   -0.548163    0.000000
    5          1           0        0.418011   -1.523509    0.000000
    6          1           0       -1.208711   -0.612420    0.000000
    7          6           0       -2.201051   -4.293130    0.000000
    8          1           0       -1.727182   -5.294044    0.000000
    9          1           0       -3.308438   -4.282761    0.000000
   10          8           0        2.010858    4.566383    0.000000
   11          8           0        0.483983    0.501800    0.000000
   12          8           0       -1.552858   -3.280166    0.000000
---------------------------------------------------------------------
                Distance matrix (angstroms):
                     1        2        3        4        5
    1  C    0.000000
    2  H    1.108163   0.000000
    3  H    1.108526   1.863631   0.000000
    4  C    4.332459   3.864151   3.829740   0.000000
    5  H    5.103725   4.447200   4.760938   1.106271   0.000000
    6  H    4.919215   4.654576   4.202894   1.106540   1.864487
    7  C    8.610402   8.138711   7.992644   4.292113   3.811862
    8  H    9.343132   8.773691   8.811558   5.015773   4.338063
    9  H    9.140495   8.780168   8.419424   4.920914   4.636798
   10  O    1.202238   2.029192   2.028780   5.534561   6.294755
   11  O    3.139986   2.675755   2.735254   1.203409   2.026383
   12  O    7.417252   6.936118   6.826388   3.092397   2.640108
                6        7        8        9       10
    6  H    0.000000
    7  C    3.812134   0.000000
    8  H    4.710246   1.107421   0.000000
    9  H    4.228505   1.107436   1.876983   0.000000
   10  O    6.098002   9.809747  10.545187  10.324836   0.000000
   11  O    2.026500   5.495522   6.203310   6.105283   4.341910
   12  O    2.689853   1.202601   2.021409   2.021696   8.617912
               11       12
   11  O    0.000000
   12  O    4.295578   0.000000
Stoichiometry    C3H6O3
Framework group  CS[SG(C3H6O3)]
Deg. of freedom   21
Full point group                 CS      NOp   2
Largest Abelian subgroup         CS      NOp   2
Largest concise Abelian subgroup C1      NOp   1
                         Standard orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic           Coordinates (Angstroms)
Number     Number      Type             X           Y           Z
---------------------------------------------------------------------
    1          6           0       -0.901856   -3.679255    0.000000
    2          1           0       -1.700861   -2.911390    0.000000
    3          1           0        0.128079   -3.269299    0.000000
    4          6           0        0.000000    0.558298    0.000000
    5          1           0       -0.693495    1.420215    0.000000
    6          1           0        1.073712    0.825832    0.000000
    7          6           0        1.367916    4.626596    0.000000
    8          1           0        0.717040    5.522554    0.000000
    9          1           0        2.458102    4.821294    0.000000
   10          8           0       -1.132093   -4.859241    0.000000
   11          8           0       -0.383606   -0.582332    0.000000
```

```
 12        8           0       0.918332    3.511193    0.000000
---------------------------------------------------------------------
Rotational constants (GHZ):     72.1313643      0.4387789      0.4361259
Isotopes: C-12,H-1,H-1,C-12,H-1,H-1,C-12,H-1,H-1,O-16,O-16,O-16
Standard basis: CBSB7 (5D, 7F)
There are   108 symmetry adapted basis functions of A'  symmetry.
There are    36 symmetry adapted basis functions of A"  symmetry.
Crude estimate of integral set expansion from redundant integrals=1.000.
Integral buffers will be    262144 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
  144 basis functions      240 primitive gaussians
   24 alpha electrons       24 beta electrons
     nuclear repulsion energy       175.7544948937 Hartrees.
One-electron integrals computed using PRISM.
NBasis=   144 RedAO= T  NBF=   108    36
NBsUse=   144 1.00D-04 NBFU=   108    36
Initial guess read from the read-write file:
Initial guess orbital symmetries:
     Occupied  (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A') (A') (A') (A") (A")
               (A") (A') (A') (A')
     Virtual   (A") (A") (A") (A') (A') (A') (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A") (A') (A") (A') (A")
               (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
               (A') (A") (A") (A") (A') (A') (A') (A') (A") (A')
               (A") (A") (A") (A') (A") (A") (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
               (A") (A") (A") (A") (A") (A") (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A') (A') (A') (A') (A")
               (A') (A') (A") (A") (A") (A') (A") (A') (A") (A')
               (A") (A") (A') (A") (A') (A') (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A") (A") (A") (A') (A')
               (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
Requested convergence on RMS density matrix=1.00D-08 within  64 cycles.
Requested convergence on MAX density matrix=1.00D-06.
SCF Done:  E(RB+HF-LYP) =  -343.617680765     A.U. after    8 cycles
          Convg  =    0.4787D-08           -V/T =  2.0031
          S**2   =   0.0000
***** Axes restored to original set *****
---------------------------------------------------------------------
Center     Atomic                 Forces (Hartrees/Bohr)
Number     Number           X              Y              Z
---------------------------------------------------------------------
   1        6        -0.000167383   -0.000755521    0.000000000
   2        1        -0.000023814    0.000377246    0.000000000
   3        1         0.000222484    0.000137968    0.000000000
   4        6        -0.000049553   -0.000371425    0.000000000
   5        1         0.000134085    0.000176270    0.000000000
   6        1        -0.000023273    0.000093854    0.000000000
   7        6         0.000769660    0.001119724    0.000000000
   8        1         0.000181434   -0.000253734    0.000000000
   9        1        -0.000315862    0.000052323    0.000000000
  10        8        -0.000056331   -0.000020739    0.000000000
  11        8         0.000056409    0.000413054    0.000000000
  12        8        -0.000727857   -0.000969021    0.000000000
---------------------------------------------------------------------
Cartesian Forces:  Max     0.001119724 RMS     0.000361371

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Internal  Forces:  Max     0.001115791 RMS     0.000184971
Search for a local minimum.
Step number  15 out of a maximum of  63
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Update second derivatives using information from points 10 11 12 13 14
                                                    15
Trust test= 3.34D-01 RLast= 3.15D-02 DXMaxT set to 1.00D+00
    Eigenvalues ---    0.00190   0.00230   0.00656   0.01172   0.01332
    Eigenvalues ---    0.01573   0.01914   0.03565   0.03565   0.05702
    Eigenvalues ---    0.06608   0.07770   0.08999   0.12977   0.13527
    Eigenvalues ---    0.16001   0.16683   0.17961   0.18988   0.19021
    Eigenvalues ---    0.19146   0.34046   0.35206   0.36986   0.36995
    Eigenvalues ---    0.37230   0.46503   0.80315   0.82298   2.12654
```

Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
Eigenvalues --- 1000.000001000.000001000.00000
RFO step: Lambda=-3.46991571D-06.
Quartic linear search produced a step of -0.21749.
Iteration 1 RMS(Cart)= 0.00462998 RMS(Int)= 0.00000138
Iteration 2 RMS(Cart)= 0.00000072 RMS(Int)= 0.00000118
Variable Old X -DE/DX Delta X Delta X Delta X New X
(Linear) (Quad) (Total)

R1	2.09412	-0.00029	-0.00021	0.00022	0.00001	2.09413
R2	2.09481	-0.00024	-0.00014	0.00005	-0.00010	2.09471
R3	2.27190	-0.00004	0.00003	0.00017	0.00020	2.27210
R4	5.93371	-0.00027	-0.00105	-0.01484	-0.01589	5.91782
R5	5.05644	0.00007	-0.00217	-0.01045	-0.01262	5.04382
R6	5.16888	-0.00006	0.00099	-0.01659	-0.01559	5.15329
R7	2.09055	-0.00007	-0.00008	0.00009	0.00001	2.09056
R8	2.09106	0.00003	0.00000	-0.00009	-0.00009	2.09097
R9	2.27411	0.00015	0.00005	-0.00001	0.00004	2.27416
R10	5.84378	-0.00005	-0.00374	-0.00443	-0.00818	5.83560
R11	4.98908	0.00013	-0.00431	-0.00214	-0.00645	4.98263
R12	5.08308	0.00002	-0.00237	-0.00632	-0.00869	5.07440
R13	2.09272	0.00031	0.00018	-0.00040	-0.00021	2.09251
R14	2.09275	0.00032	0.00019	-0.00041	-0.00022	2.09253
R15	2.27259	-0.00112	-0.00022	0.00054	0.00032	2.27291
A1	1.99725	0.00020	0.00034	0.00046	0.00079	1.99804
A2	2.14363	-0.00008	-0.00013	-0.00038	-0.00051	2.14311
A3	2.14231	-0.00012	-0.00020	-0.00008	-0.00028	2.14203
A4	3.11470	0.00005	-0.00075	0.00137	0.00062	3.11533
A5	2.00414	0.00011	0.00015	-0.00006	0.00009	2.00423
A6	2.13963	-0.00005	-0.00007	0.00002	-0.00005	2.13958
A7	2.13942	-0.00005	-0.00008	0.00004	-0.00004	2.13938
A8	2.02233	0.00007	-0.00002	0.00026	0.00024	2.02257
A9	2.13018	-0.00004	0.00001	-0.00012	-0.00012	2.13006
A10	2.13067	-0.00003	0.00001	-0.00014	-0.00012	2.13055
A11	2.98297	0.00003	-0.00017	0.00062	0.00044	2.98342
A12	0.70290	-0.00005	0.00008	0.00213	0.00222	0.70512
A13	2.95130	0.00000	0.00020	-0.00184	-0.00164	2.94966
A14	2.62899	0.00005	-0.00029	-0.00029	-0.00058	2.62841
A15	0.71451	0.00001	0.00051	0.00063	0.00114	0.71565
A16	2.86803	-0.00003	0.00004	-0.00113	-0.00109	2.86694
A17	2.70065	0.00003	-0.00055	0.00049	-0.00005	2.70059
A18	3.16451	-0.00002	0.00047	-0.00102	-0.00055	3.16396
A19	3.05996	0.00004	-0.00025	0.00070	0.00046	3.06041
A20	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
A21	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D1	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D2	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D4	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D5	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D6	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D7	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D8	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D9	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D10	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D11	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D12	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D13	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D14	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D15	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D16	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D17	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

Item Value Threshold Converged?
Maximum Force 0.001116 0.000450 NO
RMS Force 0.000185 0.000300 YES
Maximum Displacement 0.012794 0.001800 NO
RMS Displacement 0.004630 0.001200 NO
Predicted change in Energy=-1.823200D-06
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.564173	3.442428	0.000000
2	1	0	2.208310	2.540696	0.000000
3	1	0	0.476285	3.229782	0.000000
4	6	0	-0.102924	-0.547433	0.000000
5	1	0	0.419579	-1.522541	0.000000
6	1	0	-1.207525	-0.612100	0.000000
7	6	0	-2.198051	-4.288727	0.000000
8	1	0	-1.723793	-5.289332	0.000000
9	1	0	-3.305323	-4.278575	0.000000
10	8	0	2.008134	4.559803	0.000000
11	8	0	0.484678	0.502791	0.000000
12	8	0	-1.550091	-3.275414	0.000000

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	H	1.108167	0.000000			
3	H	1.108475	1.864068	0.000000		
4	C	4.324143	3.857246	3.821366	0.000000	
5	H	5.095195	4.439533	4.752661	1.106275	0.000000
6	H	4.911365	4.648446	4.194672	1.106492	1.864503
7	C	8.597970	8.127548	7.979978	4.287987	3.808382
8	H	9.330293	8.761893	8.798616	5.011269	4.333908
9	H	9.128301	8.769413	8.406901	4.916989	4.633641
10	O	1.202343	2.029006	2.028674	5.526340	6.286368
11	O	3.131577	2.669075	2.727003	1.203432	2.026378
12	O	7.404596	6.924790	6.813499	3.088069	2.636696

		6	7	8	9	10
6	H	0.000000				
7	C	3.807720	0.000000			
8	H	4.705639	1.107308	0.000000		
9	H	4.224192	1.107319	1.876930	0.000000	
10	O	6.090078	9.797371	10.532462	10.312602	0.000000
11	O	2.026458	5.491419	6.198874	6.101277	4.333620
12	O	2.685255	1.202770	2.021395	2.021676	8.605324

		11	12
11	O	0.000000	
12	O	4.291284	0.000000

Stoichiometry C3H6O3
Framework group CS[SG(C3H6O3)]
Deg. of freedom 21
Full point group CS NOp 2
Largest Abelian subgroup CS NOp 2
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.903040	-3.671756	0.000000
2	1	0	-1.702363	-2.904216	0.000000
3	1	0	0.127005	-3.262213	0.000000
4	6	0	0.000000	0.557042	0.000000
5	1	0	-0.693300	1.419121	0.000000
6	1	0	1.073750	0.824221	0.000000
7	6	0	1.369555	4.620433	0.000000
8	1	0	0.718974	5.516467	0.000000
9	1	0	2.459723	4.814569	0.000000
10	8	0	-1.133418	-4.851821	0.000000
11	8	0	-0.383935	-0.583503	0.000000
12	8	0	0.919492	3.505042	0.000000

Rotational constants (GHZ): 72.1561489 0.4400116 0.4373447
Isotopes: C-12,H-1,H-1,C-12,H-1,H-1,C-12,H-1,H-1,O-16,O-16,O-16
Standard basis: CBSB7 (5D, 7F)
There are 108 symmetry adapted basis functions of A' symmetry.
There are 36 symmetry adapted basis functions of A" symmetry.
Crude estimate of integral set expansion from redundant integrals=1.000.
Integral buffers will be 262144 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.

```
 144 basis functions      240 primitive gaussians
  24 alpha electrons       24 beta electrons
    nuclear repulsion energy       175.8786804987 Hartrees.
One-electron integrals computed using PRISM.
NBasis=   144 RedAO= T  NBF=   108    36
NBsUse=   144 1.00D-04 NBFU=   108    36
Initial guess read from the read-write file:
Initial guess orbital symmetries:
    Occupied  (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
          (A') (A') (A') (A') (A') (A') (A') (A') (A") (A")
          (A") (A') (A') (A')
    Virtual   (A") (A") (A") (A') (A') (A') (A') (A') (A') (A')
          (A') (A') (A') (A') (A') (A") (A') (A") (A') (A")
          (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
          (A') (A") (A") (A") (A') (A') (A') (A') (A") (A')
          (A") (A") (A") (A') (A") (A") (A') (A') (A') (A')
          (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
          (A") (A") (A") (A") (A") (A") (A') (A') (A') (A')
          (A') (A') (A') (A') (A') (A') (A') (A') (A') (A")
          (A') (A') (A") (A") (A") (A') (A") (A') (A") (A')
          (A") (A") (A') (A") (A') (A') (A') (A') (A') (A')
          (A') (A') (A') (A') (A') (A") (A") (A") (A') (A')
          (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
Requested convergence on RMS density matrix=1.00D-08 within  64 cycles.
Requested convergence on MAX density matrix=1.00D-06.
SCF Done:  E(RB+HF-LYP) =  -343.617683542     A.U. after    7 cycles
         Convg  =    0.3718D-08           -V/T =  2.0031
         S**2   =   0.0000
***** Axes restored to original set *****
-------------------------------------------------------------------
Center     Atomic                 Forces (Hartrees/Bohr)
Number     Number           X           Y           Z
-------------------------------------------------------------------
  1        6        -0.000031393   -0.000534273    0.000000000
  2        1        -0.000112443    0.000359720    0.000000000
  3        1         0.000248038    0.000077101    0.000000000
  4        6        -0.000010941   -0.000345381    0.000000000
  5        1         0.000120356    0.000189793    0.000000000
  6        1        -0.000030317    0.000085773    0.000000000
  7        6         0.000935598    0.001377632    0.000000000
  8        1         0.000193832   -0.000301163    0.000000000
  9        1        -0.000366238    0.000042942    0.000000000
 10        8        -0.000106810   -0.000105765    0.000000000
 11        8         0.000033896    0.000356736    0.000000000
 12        8        -0.000873578   -0.001203114    0.000000000
-------------------------------------------------------------------
Cartesian Forces:  Max     0.001377632 RMS     0.000410732

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Internal  Forces:  Max     0.001354136 RMS     0.000214383
Search for a local minimum.
Step number  16 out of a maximum of  63
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Update second derivatives using information from points 10 11 12 13 14
                                    15 16
Trust test= 1.52D+00 RLast= 2.92D-02 DXMaxT set to 1.00D+00
    Eigenvalues ---    0.00155   0.00230   0.00373   0.01172   0.01333
    Eigenvalues ---    0.01573   0.01914   0.03565   0.03565   0.05709
    Eigenvalues ---    0.06596   0.07783   0.08675   0.11779   0.13419
    Eigenvalues ---    0.16001   0.16739   0.17881   0.18986   0.19025
    Eigenvalues ---    0.19147   0.34006   0.35159   0.36981   0.36994
    Eigenvalues ---    0.37230   0.46181   0.80282   0.81574   2.43113
    Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
    Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
    Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
    Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
    Eigenvalues --- 1000.000001000.000001000.00000
RFO step:  Lambda=-4.07245599D-06.
Quartic linear search produced a step of  2.00000.
Iteration  1 RMS(Cart)=  0.01006691 RMS(Int)=  0.00001162
Iteration  2 RMS(Cart)=  0.00001024 RMS(Int)=  0.00000710
Iteration  3 RMS(Cart)=  0.00000000 RMS(Int)=  0.00000710
Variable      Old X    -DE/DX   Delta X   Delta X   Delta X     New X
```

		(Linear)	(Quad)	(Total)		
R1	2.09413	-0.00033	0.00002	0.00028	0.00029	2.09442
R2	2.09471	-0.00025	-0.00019	0.00012	-0.00008	2.09463
R3	2.27210	-0.00014	0.00040	-0.00012	0.00027	2.27237
R4	5.91782	-0.00020	-0.03178	-0.00731	-0.03910	5.87872
R5	5.04382	0.00006	-0.02525	-0.00049	-0.02572	5.01810
R6	5.15329	-0.00007	-0.03118	-0.01571	-0.04688	5.10640
R7	2.09056	-0.00009	0.00002	0.00012	0.00014	2.09070
R8	2.09097	0.00004	-0.00018	-0.00001	-0.00019	2.09078
R9	2.27416	0.00015	0.00009	-0.00010	-0.00001	2.27415
R10	5.83560	-0.00002	-0.01636	0.00870	-0.00766	5.82795
R11	4.98263	0.00013	-0.01290	0.01275	-0.00014	4.98249
R12	5.07440	0.00002	-0.01738	0.00295	-0.01443	5.05997
R13	2.09251	0.00035	-0.00043	-0.00016	-0.00058	2.09193
R14	2.09253	0.00037	-0.00044	-0.00017	-0.00061	2.09192
R15	2.27291	-0.00135	0.00064	0.00013	0.00077	2.27367
A1	1.99804	0.00011	0.00159	-0.00112	0.00046	1.99850
A2	2.14311	-0.00002	-0.00103	0.00046	-0.00056	2.14256
A3	2.14203	-0.00009	-0.00056	0.00065	0.00010	2.14213
A4	3.11533	0.00006	0.00125	0.00364	0.00488	3.12021
A5	2.00423	0.00009	0.00018	-0.00026	-0.00008	2.00415
A6	2.13958	-0.00004	-0.00011	0.00005	-0.00006	2.13952
A7	2.13938	-0.00005	-0.00007	0.00021	0.00014	2.13952
A8	2.02257	0.00006	0.00048	-0.00004	0.00044	2.02301
A9	2.13006	-0.00004	-0.00024	0.00002	-0.00021	2.12985
A10	2.13055	-0.00002	-0.00025	0.00002	-0.00023	2.13032
A11	2.98342	0.00003	0.00089	0.00108	0.00197	2.98538
A12	0.70512	-0.00007	0.00444	0.00106	0.00554	0.71066
A13	2.94966	0.00001	-0.00328	-0.00195	-0.00525	2.94441
A14	2.62841	0.00006	-0.00116	0.00089	-0.00029	2.62812
A15	0.71565	0.00000	0.00228	-0.00116	0.00112	0.71677
A16	2.86694	-0.00003	-0.00218	-0.00102	-0.00320	2.86375
A17	2.70059	0.00003	-0.00011	0.00218	0.00207	2.70267
A18	3.16396	-0.00002	-0.00110	-0.00232	-0.00342	3.16055
A19	3.06041	0.00004	0.00091	0.00138	0.00230	3.06271
A20	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
A21	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D1	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D2	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D4	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D5	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D6	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D7	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D8	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D9	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D10	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D11	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D12	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D13	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D14	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D15	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D16	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D17	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

Item	Value	Threshold	Converged?
Maximum Force	0.001354	0.000450	NO
RMS Force	0.000214	0.000300	YES
Maximum Displacement	0.036282	0.001800	NO
RMS Displacement	0.010070	0.001200	NO

Predicted change in Energy=-5.108721D-06

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.558182	3.428702	0.000000
2	1	0	2.207407	2.530437	0.000000
3	1	0	0.471436	3.210520	0.000000
4	6	0	-0.099261	-0.543072	0.000000
5	1	0	0.425361	-1.517126	0.000000
6	1	0	-1.203617	-0.610181	0.000000
7	6	0	-2.195372	-4.279819	0.000000

```
  8        1           0     -1.720071   -5.279588    0.000000
  9        1           0     -3.302330   -4.270482    0.000000
 10        8           0      1.996607    4.548417    0.000000
 11        8           0      0.486152    0.508367    0.000000
 12        8           0     -1.548166   -3.265542    0.000000
---------------------------------------------------------------------
             Distance matrix (angstroms):
                  1        2        3        4        5
  1  C    0.000000
  2  H    1.108319   0.000000
  3  H    1.108432   1.864432   0.000000
  4  C    4.303732   3.842808   3.796729   0.000000
  5  H    5.073903   4.422494   4.727870   1.106350   0.000000
  6  H    4.892863   4.636654   4.171757   1.106392   1.864434
  7  C    8.573824   8.109503   7.950914   4.284502   3.807980
  8  H    9.304905   8.741944   8.768389   5.006157   4.331166
  9  H    9.105054   8.752697   8.378944   4.914594   4.634291
 10  O    1.202488   2.028960   2.028821   5.505990   6.265750
 11  O    3.110884   2.655463   2.702193   1.203426   2.026405
 12  O    7.379857   6.906352   6.783669   3.084018   2.636620
                  6        7        8        9       10
  6  H    0.000000
  7  C    3.801292   0.000000
  8  H    4.697881   1.107001   0.000000
  9  H    4.219289   1.106997   1.876656   0.000000
 10  O    6.070632   9.772944  10.507301  10.288426   0.000000
 11  O    2.026443   5.487923   6.194179   6.098360   4.313174
 12  O    2.677621   1.203176   2.021370   2.021632   8.580406
                 11       12
 11  O    0.000000
 12  O    4.287288   0.000000
Stoichiometry    C3H6O3
Framework group  CS[SG(C3H6O3)]
Deg. of freedom   21
Full point group                 CS     NOp   2
Largest Abelian subgroup         CS     NOp   2
Largest concise Abelian subgroup C1     NOp   1
                    Standard orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic           Coordinates (Angstroms)
Number     Number      Type             X         Y         Z
---------------------------------------------------------------------
  1        6           0     -0.927066   -3.650283    0.000000
  2        1           0     -1.725253   -2.881342    0.000000
  3        1           0      0.103786   -3.242896    0.000000
  4        6           0      0.000000    0.552414    0.000000
  5        1           0     -0.688995    1.418032    0.000000
  6        1           0      1.074965    0.814242    0.000000
  7        6           0      1.400450    4.601573    0.000000
  8        1           0      0.755437    5.501244    0.000000
  9        1           0      2.491529    4.788628    0.000000
 10        8           0     -1.160041   -4.829986    0.000000
 11        8           0     -0.389740   -0.586154    0.000000
 12        8           0      0.943309    3.488624    0.000000
---------------------------------------------------------------------
Rotational constants (GHZ):     71.8675908      0.4424522      0.4397449
Isotopes: C-12,H-1,H-1,C-12,H-1,H-1,C-12,H-1,H-1,O-16,O-16,O-16
Standard basis: CBSB7 (5D, 7F)
There are   108 symmetry adapted basis functions of A'  symmetry.
There are    36 symmetry adapted basis functions of A"  symmetry.
Crude estimate of integral set expansion from redundant integrals=1.000.
Integral buffers will be    262144 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
  144 basis functions      240 primitive gaussians
   24 alpha electrons       24 beta electrons
      nuclear repulsion energy       176.1214642136 Hartrees.
One-electron integrals computed using PRISM.
NBasis=   144 RedAO= T  NBF=   108    36
NBsUse=   144 1.00D-04 NBFU=   108    36
Initial guess read from the read-write file:
Initial guess orbital symmetries:
     Occupied  (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A') (A') (A') (A") (A")
```

```
          (A") (A') (A') (A')
    Virtual   (A") (A") (A") (A') (A') (A') (A') (A') (A') (A')
          (A') (A') (A') (A') (A') (A") (A') (A") (A') (A")
          (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
          (A') (A") (A") (A") (A') (A') (A') (A') (A") (A')
          (A") (A") (A") (A') (A") (A") (A') (A') (A') (A')
          (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
          (A") (A") (A") (A") (A") (A") (A') (A') (A') (A')
          (A') (A') (A') (A') (A') (A') (A') (A') (A') (A")
          (A') (A') (A") (A") (A") (A') (A") (A') (A") (A')
          (A") (A") (A') (A") (A') (A') (A') (A') (A') (A')
          (A') (A') (A') (A') (A') (A") (A") (A") (A') (A')
          (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
Requested convergence on RMS density matrix=1.00D-08 within  64 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Integral accuracy reduced to 1.0D-05 until final iterations.
Initial convergence to 1.0D-05 achieved.  Increase integral accuracy.
SCF Done:  E(RB+HF-LYP) =  -343.617687494     A.U. after    9 cycles
         Convg  =    0.3899D-08           -V/T =  2.0031
         S**2   =   0.0000
***** Axes restored to original set *****
-------------------------------------------------------------------
Center     Atomic                 Forces (Hartrees/Bohr)
Number     Number           X           Y           Z
-------------------------------------------------------------------
  1        6         0.000155539  -0.000294435   0.000000000
  2        1        -0.000246130   0.000418609   0.000000000
  3        1         0.000324683   0.000062986   0.000000000
  4        6         0.000001563  -0.000423294   0.000000000
  5        1         0.000105855   0.000230219   0.000000000
  6        1        -0.000048406   0.000096362   0.000000000
  7        6         0.001345515   0.002021671   0.000000000
  8        1         0.000246760  -0.000434683   0.000000000
  9        1        -0.000515299   0.000032174   0.000000000
 10        8        -0.000182927  -0.000235208   0.000000000
 11        8         0.000011949   0.000258283   0.000000000
 12        8        -0.001199104  -0.001732683   0.000000000
-------------------------------------------------------------------
Cartesian Forces:  Max     0.002021671 RMS     0.000570593

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Internal  Forces:  Max     0.001944192 RMS     0.000301285
Search for a local minimum.
Step number  17 out of a maximum of  63
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Update second derivatives using information from points 10 11 12 13 14
                                    15 16 17
Trust test= 7.74D-01 RLast= 6.91D-02 DXMaxT set to 1.00D+00
    Eigenvalues ---    0.00150   0.00230   0.00328   0.01172   0.01338
    Eigenvalues ---    0.01573   0.01914   0.03565   0.03565   0.05726
    Eigenvalues ---    0.06559   0.07800   0.08344   0.11253   0.13384
    Eigenvalues ---    0.16001   0.16765   0.17833   0.18985   0.19026
    Eigenvalues ---    0.19142   0.34010   0.35118   0.36979   0.36994
    Eigenvalues ---    0.37230   0.45259   0.80260   0.81353   2.15169
    Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
    Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
    Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
    Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
    Eigenvalues --- 1000.000001000.000001000.00000
RFO step:  Lambda=-4.16040128D-06.
Quartic linear search produced a step of  0.03546.
Iteration  1 RMS(Cart)=  0.00291771 RMS(Int)=  0.00000340
Iteration  2 RMS(Cart)=  0.00000359 RMS(Int)=  0.00000076
Iteration  3 RMS(Cart)=  0.00000000 RMS(Int)=  0.00000076
Variable      Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                        (Linear)    (Quad)   (Total)
   R1       2.09442  -0.00043   0.00001  -0.00008  -0.00006   2.09436
   R2       2.09463  -0.00030   0.00000  -0.00016  -0.00017   2.09447
   R3       2.27237  -0.00029   0.00001  -0.00006  -0.00005   2.27232
   R4       5.87872  -0.00009  -0.00139  -0.00264  -0.00402   5.87469
   R5       5.01810   0.00007  -0.00091   0.00388   0.00297   5.02107
   R6       5.10640  -0.00004  -0.00166  -0.00913  -0.01079   5.09561
   R7       2.09070  -0.00012   0.00000   0.00001   0.00002   2.09072
```

R8	2.09078	0.00006	-0.00001	-0.00002	-0.00002	2.09076
R9	2.27415	0.00021	0.00000	0.00000	0.00000	2.27415
R10	5.82795	-0.00001	-0.00027	0.01033	0.01006	5.83800
R11	4.98249	0.00014	-0.00001	0.01424	0.01423	4.99673
R12	5.05997	0.00004	-0.00051	0.00569	0.00518	5.06515
R13	2.09193	0.00050	-0.00002	0.00017	0.00015	2.09208
R14	2.09192	0.00052	-0.00002	0.00017	0.00015	2.09207
R15	2.27367	-0.00194	0.00003	-0.00025	-0.00023	2.27345
A1	1.99850	0.00002	0.00002	-0.00014	-0.00012	1.99838
A2	2.14256	0.00005	-0.00002	0.00001	-0.00001	2.14254
A3	2.14213	-0.00007	0.00000	0.00013	0.00014	2.14226
A4	3.12021	0.00007	0.00017	0.00312	0.00330	3.12351
A5	2.00415	0.00009	0.00000	0.00031	0.00030	2.00445
A6	2.13952	-0.00005	0.00000	-0.00024	-0.00024	2.13927
A7	2.13952	-0.00004	0.00000	-0.00006	-0.00006	2.13946
A8	2.02301	0.00004	0.00002	0.00005	0.00007	2.02308
A9	2.12985	-0.00003	-0.00001	-0.00004	-0.00005	2.12980
A10	2.13032	-0.00001	-0.00001	-0.00002	-0.00002	2.13030
A11	2.98538	0.00004	0.00007	0.00090	0.00097	2.98636
A12	0.71066	-0.00013	0.00020	0.00037	0.00056	0.71122
A13	2.94441	0.00004	-0.00019	-0.00138	-0.00156	2.94285
A14	2.62812	0.00009	-0.00001	0.00101	0.00100	2.62912
A15	0.71677	0.00000	0.00004	-0.00138	-0.00134	0.71543
A16	2.86375	-0.00003	-0.00011	-0.00068	-0.00079	2.86296
A17	2.70267	0.00003	0.00007	0.00206	0.00213	2.70480
A18	3.16055	-0.00001	-0.00012	-0.00200	-0.00212	3.15842
A19	3.06271	0.00004	0.00008	0.00118	0.00127	3.06397
A20	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
A21	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D1	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D2	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D4	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D5	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D6	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D7	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D8	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D9	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D10	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D11	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D12	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D13	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D14	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D15	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D16	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D17	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

Item	Value	Threshold	Converged?
Maximum Force	0.001944	0.000450	NO
RMS Force	0.000301	0.000300	NO
Maximum Displacement	0.007355	0.001800	NO
RMS Displacement	0.002918	0.001200	NO

Predicted change in Energy=-2.082903D-06

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.559505	3.428454	0.000000
2	1	0	2.211823	2.532476	0.000000
3	1	0	0.473636	3.206386	0.000000
4	6	0	-0.095537	-0.542160	0.000000
5	1	0	0.430432	-1.515499	0.000000
6	1	0	-1.199807	-0.610457	0.000000
7	6	0	-2.196497	-4.282246	0.000000
8	1	0	-1.720840	-5.281934	0.000000
9	1	0	-3.303535	-4.273188	0.000000
10	8	0	1.994044	4.549652	0.000000
11	8	0	0.488684	0.509945	0.000000
12	8	0	-1.549636	-3.267891	0.000000

Distance matrix (angstroms):

	1	2	3	4	5

```
  1  C    0.000000
  2  H    1.108285   0.000000
  3  H    1.108344   1.864256   0.000000
  4  C    4.301737   3.844125   3.791511   0.000000
  5  H    5.071241   4.422608   4.722083   1.106360   0.000000
  6  H    4.891483   4.638669   4.167577   1.106381   1.864613
  7  C    8.576856   8.116263   7.950423   4.289788   3.815186
  8  H    9.307606   8.748191   8.767400   5.010695   4.337511
  9  H    9.108483   8.759922   8.379203   4.920551   4.641913
 10  O    1.202460   2.028898   2.028794   5.503899   6.263461
 11  O    3.108755   2.657036   2.696483   1.203428   2.026281
 12  O    7.382940   6.913236   6.783059   3.089339   2.644153
                6          7          8          9         10
  6  H    0.000000
  7  C    3.804659   0.000000
  8  H    4.700444   1.107079   0.000000
  9  H    4.223893   1.107076   1.876831   0.000000
 10  O    6.068559   9.775636  10.510017  10.291106   0.000000
 11  O    2.026401   5.493204   6.199021   6.104039   4.311072
 12  O    2.680362   1.203057   2.021306   2.021580   8.583219
               11         12
 11  O    0.000000
 12  O    4.292644   0.000000
Stoichiometry    C3H6O3
Framework group  CS[SG(C3H6O3)]
Deg. of freedom   21
Full point group                 CS     NOp   2
Largest Abelian subgroup         CS     NOp   2
Largest concise Abelian subgroup C1     NOp   1
                  Standard orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic           Coordinates (Angstroms)
Number     Number      Type             X           Y           Z
---------------------------------------------------------------------
   1         6          0       -0.947352   -3.645429    0.000000
   2         1          0       -1.744071   -2.875017    0.000000
   3         1          0        0.084131   -3.239881    0.000000
   4         6          0        0.000000    0.550696    0.000000
   5         1          0       -0.685560    1.419050    0.000000
   6         1          0        1.076062    0.807930    0.000000
   7         6          0        1.426279    4.596436    0.000000
   8         1          0        0.785748    5.499400    0.000000
   9         1          0        2.518374    4.777943    0.000000
  10         8          0       -1.182547   -4.824662    0.000000
  11         8          0       -0.394531   -0.586222    0.000000
  12         8          0        0.963548    3.485929    0.000000
---------------------------------------------------------------------
Rotational constants (GHZ):     71.5267369      0.4421663      0.4394497
Isotopes: C-12,H-1,H-1,C-12,H-1,H-1,C-12,H-1,H-1,O-16,O-16,O-16
Standard basis: CBSB7 (5D, 7F)
There are   108 symmetry adapted basis functions of A'  symmetry.
There are    36 symmetry adapted basis functions of A"  symmetry.
Crude estimate of integral set expansion from redundant integrals=1.000.
Integral buffers will be    262144 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
  144 basis functions      240 primitive gaussians
   24 alpha electrons       24 beta electrons
      nuclear repulsion energy       176.0907848583 Hartrees.
One-electron integrals computed using PRISM.
NBasis=   144 RedAO= T  NBF=   108    36
NBsUse=   144 1.00D-04 NBFU=   108    36
Initial guess read from the read-write file:
Initial guess orbital symmetries:
     Occupied  (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A') (A') (A') (A") (A")
               (A") (A') (A') (A')
     Virtual   (A") (A") (A") (A') (A') (A') (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A") (A') (A") (A') (A")
               (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
               (A') (A") (A") (A") (A') (A') (A') (A') (A") (A')
               (A") (A") (A") (A') (A") (A") (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
               (A") (A") (A") (A") (A") (A") (A') (A') (A') (A')
```

(A') (A') (A') (A') (A') (A') (A') (A') (A') (A")
(A') (A') (A") (A") (A") (A') (A") (A') (A") (A')
(A") (A") (A') (A") (A') (A') (A') (A') (A') (A')
(A') (A') (A') (A') (A') (A") (A") (A") (A') (A')
(A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
Requested convergence on RMS density matrix=1.00D-08 within 64 cycles.
Requested convergence on MAX density matrix=1.00D-06.
SCF Done: E(RB+HF-LYP) = -343.617691161 A.U. after 8 cycles
Convg = 0.2673D-08 -V/T = 2.0031
S**2 = 0.0000
***** Axes restored to original set *****

Center Atomic Forces (Hartrees/Bohr)
Number Number X Y Z
---
1 6 0.000133740 -0.000303453 0.000000000
2 1 -0.000219243 0.000390645 0.000000000
3 1 0.000292224 0.000069797 0.000000000
4 6 -0.000004257 -0.000414158 0.000000000
5 1 0.000086484 0.000200018 0.000000000
6 1 -0.000047736 0.000077000 0.000000000
7 6 0.001242369 0.001863576 0.000000000
8 1 0.000216755 -0.000410248 0.000000000
9 1 -0.000479206 0.000016262 0.000000000
10 8 -0.000154542 -0.000186693 0.000000000
11 8 0.000008586 0.000237917 0.000000000
12 8 -0.001075175 -0.001540663 0.000000000

Cartesian Forces: Max 0.001863576 RMS 0.000520010

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Internal Forces: Max 0.001765895 RMS 0.000274065
Search for a local minimum.
Step number 18 out of a maximum of 63
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Update second derivatives using information from points 10 11 12 13 14
15 16 17 18
Trust test= 1.76D+00 RLast= 2.24D-02 DXMaxT set to 1.00D+00
Eigenvalues --- 0.00143 0.00171 0.00230 0.01173 0.01337
Eigenvalues --- 0.01573 0.01916 0.03565 0.03565 0.05727
Eigenvalues --- 0.06571 0.07789 0.08350 0.11153 0.13364
Eigenvalues --- 0.16000 0.16866 0.17678 0.18986 0.19022
Eigenvalues --- 0.19124 0.33878 0.35008 0.36944 0.36995
Eigenvalues --- 0.37230 0.37719 0.80229 0.81169 1.16180
Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
Eigenvalues --- 1000.000001000.000001000.00000
RFO step: Lambda=-3.63013895D-06.
Quartic linear search produced a step of 2.00000.
Iteration 1 RMS(Cart)= 0.00448552 RMS(Int)= 0.00000861
Iteration 2 RMS(Cart)= 0.00000840 RMS(Int)= 0.00000371
Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000371
Variable Old X -DE/DX Delta X Delta X Delta X New X
(Linear) (Quad) (Total)
R1 2.09436 -0.00040 -0.00013 -0.00089 -0.00101 2.09334
R2 2.09447 -0.00027 -0.00033 -0.00055 -0.00088 2.09359
R3 2.27232 -0.00023 -0.00011 0.00000 -0.00011 2.27221
R4 5.87469 -0.00008 -0.00805 0.00293 -0.00512 5.86957
R5 5.02107 0.00007 0.00595 0.00037 0.00632 5.02739
R6 5.09561 -0.00002 -0.02158 0.00689 -0.01469 5.08093
R7 2.09072 -0.00011 0.00004 -0.00029 -0.00025 2.09047
R8 2.09076 0.00005 -0.00004 0.00009 0.00005 2.09080
R9 2.27415 0.00021 0.00001 0.00021 0.00022 2.27437
R10 5.83800 -0.00002 0.02011 -0.00473 0.01538 5.85338
R11 4.99673 0.00012 0.02847 -0.00568 0.02279 5.01952
R12 5.06515 0.00002 0.01036 -0.00202 0.00834 5.07349
R13 2.09208 0.00046 0.00030 0.00104 0.00134 2.09342
R14 2.09207 0.00048 0.00030 0.00108 0.00138 2.09344
R15 2.27345 -0.00177 -0.00045 -0.00123 -0.00168 2.27177
A1 1.99838 0.00002 -0.00025 0.00069 0.00045 1.99882
A2 2.14254 0.00004 -0.00002 -0.00011 -0.00013 2.14241

A3	2.14226	-0.00006	0.00027	-0.00058	-0.00031	2.14195
A4	3.12351	0.00007	0.00659	-0.00138	0.00521	3.12872
A5	2.00445	0.00008	0.00060	0.00054	0.00114	2.00559
A6	2.13927	-0.00004	-0.00049	-0.00026	-0.00074	2.13853
A7	2.13946	-0.00004	-0.00012	-0.00028	-0.00040	2.13906
A8	2.02308	0.00002	0.00014	-0.00038	-0.00024	2.02284
A9	2.12980	-0.00002	-0.00009	0.00018	0.00009	2.12989
A10	2.13030	0.00000	-0.00005	0.00021	0.00016	2.13046
A11	2.98636	0.00004	0.00194	-0.00034	0.00161	2.98796
A12	0.71122	-0.00012	0.00112	-0.00065	0.00046	0.71167
A13	2.94285	0.00003	-0.00312	0.00083	-0.00228	2.94057
A14	2.62912	0.00008	0.00200	-0.00019	0.00182	2.63094
A15	0.71543	0.00000	-0.00268	0.00065	-0.00202	0.71341
A16	2.86296	-0.00003	-0.00158	0.00025	-0.00133	2.86163
A17	2.70480	0.00003	0.00426	-0.00091	0.00335	2.70815
A18	3.15842	-0.00001	-0.00425	0.00090	-0.00335	3.15507
A19	3.06397	0.00004	0.00253	-0.00047	0.00206	3.06604
A20	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
A21	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D1	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D2	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D4	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D5	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D6	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D7	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D8	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D9	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D10	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D11	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D12	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D13	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D14	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D15	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D16	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D17	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

Item	Value	Threshold	Converged?
Maximum Force	0.001766	0.000450	NO
RMS Force	0.000274	0.000300	YES
Maximum Displacement	0.011115	0.001800	NO
RMS Displacement	0.004486	0.001200	NO

Predicted change in Energy=-3.425400D-06

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.560503	3.428785	0.000000
2	1	0	2.217444	2.536858	0.000000
3	1	0	0.476232	3.201299	0.000000
4	6	0	-0.091252	-0.540623	0.000000
5	1	0	0.437114	-1.512513	0.000000
6	1	0	-1.195450	-0.610457	0.000000
7	6	0	-2.199307	-4.285190	0.000000
8	1	0	-1.722926	-5.285320	0.000000
9	1	0	-3.307079	-4.276859	0.000000
10	8	0	1.988969	4.552258	0.000000
11	8	0	0.491143	0.512628	0.000000
12	8	0	-1.553437	-3.271258	0.000000

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	H	1.107748	0.000000			
3	H	1.107878	1.863680	0.000000		
4	C	4.299360	3.847202	3.784708	0.000000	
5	H	5.067389	4.423458	4.713974	1.106228	0.000000
6	H	4.889863	4.642568	4.162211	1.106405	1.865200
7	C	8.581468	8.126994	7.950221	4.297171	3.826023
8	H	9.312172	8.758595	8.766926	5.017421	4.347396
9	H	9.114292	8.771950	8.380709	4.929605	4.654094
10	O	1.202403	2.028309	2.028168	5.501341	6.260167

```
 11  O    3.106043   2.660380   2.688712   1.203545   2.025861
 12  O    7.388316   6.924865   6.783329   3.097476   2.656215
            6          7          8          9         10
  6  H    0.000000
  7  C    3.809382   0.000000
  8  H    4.704527   1.107790   0.000000
  9  H    4.231014   1.107803   1.877906   0.000000
 10  O    6.065818   9.779680  10.514566  10.295700   0.000000
 11  O    2.026306   5.500689   6.206312   6.112747   4.308374
 12  O    2.684775   1.202167   2.021181   2.021508   8.588134
            11         12
 11  O    0.000000
 12  O    4.300942   0.000000
Stoichiometry    C3H6O3
Framework group  CS[SG(C3H6O3)]
Deg. of freedom   21
Full point group                 CS     NOp   2
Largest Abelian subgroup         CS     NOp   2
Largest concise Abelian subgroup C1     NOp   1
                     Standard orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic           Coordinates (Angstroms)
Number     Number      Type             X           Y           Z
---------------------------------------------------------------------
   1          6           0       -0.978254   -3.638122    0.000000
   2          1           0       -1.772605   -2.866038    0.000000
   3          1           0        0.054015   -3.235857    0.000000
   4          6           0        0.000000    0.548466    0.000000
   5          1           0       -0.680634    1.420520    0.000000
   6          1           0        1.077786    0.798483    0.000000
   7          6           0        1.465255    4.588108    0.000000
   8          1           0        0.831270    5.496547    0.000000
   9          1           0        2.559388    4.761605    0.000000
  10          8           0       -1.216625   -4.816660    0.000000
  11          8           0       -0.401734   -0.586052    0.000000
  12          8           0        0.994455    3.481965    0.000000
---------------------------------------------------------------------
Rotational constants (GHZ):     70.9894438      0.4416965      0.4389653
Isotopes: C-12,H-1,H-1,C-12,H-1,H-1,C-12,H-1,H-1,O-16,O-16,O-16
Standard basis: CBSB7 (5D, 7F)
There are   108 symmetry adapted basis functions of A'  symmetry.
There are    36 symmetry adapted basis functions of A"  symmetry.
Crude estimate of integral set expansion from redundant integrals=1.000.
Integral buffers will be    262144 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
  144 basis functions      240 primitive gaussians
   24 alpha electrons       24 beta electrons
     nuclear repulsion energy       176.0497308179 Hartrees.
One-electron integrals computed using PRISM.
NBasis=   144 RedAO= T  NBF=   108    36
NBsUse=   144 1.00D-04 NBFU=   108    36
Initial guess read from the read-write file:
Initial guess orbital symmetries:
     Occupied  (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A') (A') (A') (A") (A")
               (A") (A') (A') (A')
     Virtual   (A") (A") (A") (A') (A') (A') (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A") (A') (A") (A') (A")
               (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
               (A') (A") (A") (A") (A') (A') (A') (A') (A") (A')
               (A") (A") (A") (A') (A") (A") (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
               (A") (A") (A") (A") (A") (A") (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A') (A') (A') (A') (A")
               (A') (A') (A") (A") (A") (A') (A") (A') (A") (A')
               (A") (A") (A') (A") (A') (A') (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A") (A") (A") (A') (A')
               (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
Requested convergence on RMS density matrix=1.00D-08 within  64 cycles.
Requested convergence on MAX density matrix=1.00D-06.
SCF Done:  E(RB+HF-LYP) =  -343.617697735     A.U. after    8 cycles
          Convg  =    0.5335D-08           -V/T =  2.0031
          S**2   =   0.0000
```

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

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000063403	-0.000073866	0.000000000
2	1	-0.000040990	0.000110039	0.000000000
3	1	0.000070040	-0.000022011	0.000000000
4	6	0.000041735	-0.000132301	0.000000000
5	1	0.000039577	0.000066349	0.000000000
6	1	-0.000003323	0.000000690	0.000000000
7	6	0.000354633	0.000481773	0.000000000
8	1	0.000028602	-0.000119462	0.000000000
9	1	-0.000123757	-0.000025949	0.000000000
10	8	-0.000041755	-0.000020821	0.000000000
11	8	-0.000072402	0.000082565	0.000000000
12	8	-0.000315763	-0.000347006	0.000000000

Cartesian Forces: Max 0.000481773 RMS 0.000137152

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Internal Forces: Max 0.000423045 RMS 0.000068096
Search for a local minimum.
Step number 19 out of a maximum of 63
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Update second derivatives using information from points 10 11 12 13 14
15 16 17 18 19
Trust test= 1.92D+00 RLast= 3.45D-02 DXMaxT set to 1.00D+00
Eigenvalues --- 0.00141 0.00184 0.00230 0.01173 0.01336
Eigenvalues --- 0.01572 0.01920 0.03565 0.03565 0.05726
Eigenvalues --- 0.06582 0.07772 0.08298 0.10708 0.13316
Eigenvalues --- 0.15999 0.16856 0.17485 0.18986 0.19037
Eigenvalues --- 0.19133 0.32746 0.34412 0.35372 0.36989
Eigenvalues --- 0.36998 0.37230 0.79792 0.80447 1.02908
Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
Eigenvalues --- 1000.000001000.000001000.00000
RFO step: Lambda=-3.97551423D-06.
Quartic linear search produced a step of 0.88745.
Iteration 1 RMS(Cart)= 0.00948205 RMS(Int)= 0.00003913
Iteration 2 RMS(Cart)= 0.00004098 RMS(Int)= 0.00001126
Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00001126

Variable	Old X	-DE/DX (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.09334	-0.00010	-0.00090	0.00071	-0.00017	2.09317
R2	2.09359	-0.00006	-0.00078	0.00035	-0.00041	2.09318
R3	2.27221	-0.00003	-0.00009	0.00001	-0.00009	2.27212
R4	5.86957	0.00000	-0.00455	-0.01025	-0.01483	5.85474
R5	5.02739	0.00005	0.00561	0.00292	0.00853	5.03592
R6	5.08093	-0.00004	-0.01303	-0.02483	-0.03786	5.04307
R7	2.09047	-0.00003	-0.00022	0.00028	0.00006	2.09053
R8	2.09080	0.00001	0.00004	-0.00011	-0.00007	2.09074
R9	2.27437	0.00006	0.00020	-0.00015	0.00004	2.27441
R10	5.85338	0.00000	0.01365	0.01712	0.03076	5.88414
R11	5.01952	0.00006	0.02023	0.02503	0.04526	5.06478
R12	5.07349	-0.00002	0.00740	0.00645	0.01385	5.08734
R13	2.09342	0.00012	0.00119	-0.00057	0.00062	2.09404
R14	2.09344	0.00012	0.00122	-0.00060	0.00062	2.09406
R15	2.27177	-0.00042	-0.00149	0.00073	-0.00077	2.27100
A1	1.99882	-0.00001	0.00040	-0.00116	-0.00077	1.99805
A2	2.14241	0.00002	-0.00012	0.00030	0.00018	2.14259
A3	2.14195	-0.00001	-0.00028	0.00086	0.00059	2.14254
A4	3.12872	0.00004	0.00463	0.00652	0.01115	3.13987
A5	2.00559	0.00002	0.00101	-0.00025	0.00075	2.00634
A6	2.13853	0.00000	-0.00066	0.00001	-0.00064	2.13789
A7	2.13906	-0.00002	-0.00035	0.00024	-0.00010	2.13896
A8	2.02284	-0.00004	-0.00022	-0.00041	-0.00062	2.02222
A9	2.12989	0.00002	0.00008	0.00022	0.00029	2.13018
A10	2.13046	0.00002	0.00014	0.00019	0.00033	2.13079
A11	2.98796	0.00003	0.00143	0.00207	0.00350	2.99146
A12	0.71167	-0.00003	0.00040	0.00160	0.00195	0.71362

A13	2.94057	-0.00001	-0.00202	-0.00351	-0.00550	2.93507
A14	2.63094	0.00004	0.00162	0.00191	0.00355	2.63450
A15	0.71341	0.00000	-0.00180	-0.00230	-0.00410	0.70931
A16	2.86163	-0.00003	-0.00118	-0.00191	-0.00309	2.85854
A17	2.70815	0.00003	0.00298	0.00421	0.00719	2.71534
A18	3.15507	-0.00002	-0.00297	-0.00445	-0.00742	3.14766
A19	3.06604	0.00003	0.00183	0.00263	0.00446	3.07050
A20	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
A21	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D1	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D2	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D4	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D5	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D6	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D7	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D8	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D9	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D10	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D11	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D12	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D13	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D14	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D15	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D16	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D17	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

Item	Value	Threshold	Converged?
Maximum Force	0.000423	0.000450	YES
RMS Force	0.000068	0.000300	YES
Maximum Displacement	0.025620	0.001800	NO
RMS Displacement	0.009488	0.001200	NO

Predicted change in Energy=-4.207685D-06

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.561387	3.428739	0.000000
2	1	0	2.228482	2.544491	0.000000
3	1	0	0.480198	3.188022	0.000000
4	6	0	-0.081915	-0.536214	0.000000
5	1	0	0.450994	-1.505658	0.000000
6	1	0	-1.185797	-0.610371	0.000000
7	6	0	-2.205674	-4.290464	0.000000
8	1	0	-1.728384	-5.290523	0.000000
9	1	0	-3.313782	-4.283675	0.000000
10	8	0	1.976694	4.557092	0.000000
11	8	0	0.496249	0.519391	0.000000
12	8	0	-1.561098	-3.276189	0.000000

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	H	1.107659	0.000000			
3	H	1.107662	1.862962	0.000000		
4	C	4.292003	3.850802	3.766417	0.000000	
5	H	5.057790	4.423028	4.693771	1.106261	0.000000
6	H	4.884816	4.648704	4.147689	1.106370	1.865643
7	C	8.589344	8.147291	7.946172	4.313322	3.848770
8	H	9.319233	8.777484	8.761481	5.031333	4.367481
9	H	9.124067	8.794347	8.379769	4.948579	4.678773
10	O	1.202356	2.028289	2.028264	5.493599	6.251775
11	O	3.098197	2.664895	2.668680	1.203567	2.025554
12	O	7.396348	6.945591	6.778857	3.113751	2.680167

		6	7	8	9	10
6	H	0.000000				
7	C	3.818800	0.000000			
8	H	4.711499	1.108117	0.000000		
9	H	4.245172	1.108129	1.878092	0.000000	
10	O	6.058384	9.786289	10.521555	10.302830	0.000000
11	O	2.026238	5.516801	6.221261	6.130724	4.300552
12	O	2.692107	1.201762	2.021268	2.021615	8.595130

```
            11        12
  11  O    0.000000
  12  O    4.317302   0.000000
Stoichiometry    C3H6O3
Framework group  CS[SG(C3H6O3)]
Deg. of freedom   21
Full point group                 CS     NOp   2
Largest Abelian subgroup         CS     NOp   2
Largest concise Abelian subgroup C1     NOp   1
                     Standard orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic           Coordinates (Angstroms)
Number     Number      Type             X           Y           Z
---------------------------------------------------------------------
   1         6          0       -1.047712   -3.618957    0.000000
   2         1          0       -1.836590   -2.841410    0.000000
   3         1          0       -0.013166   -3.223190    0.000000
   4         6          0        0.000000    0.543205    0.000000
   5         1          0       -0.668547    1.424601    0.000000
   6         1          0        1.081277    0.777500    0.000000
   7         6          0        1.553752    4.566959    0.000000
   8         1          0        0.935767    5.486751    0.000000
   9         1          0        2.651011    4.721789    0.000000
  10         8          0       -1.294084   -4.795801    0.000000
  11         8          0       -0.418095   -0.585410    0.000000
  12         8          0        1.063930    3.469550    0.000000
---------------------------------------------------------------------
Rotational constants (GHZ):     69.8257618      0.4409712      0.4382038
Isotopes: C-12,H-1,H-1,C-12,H-1,H-1,C-12,H-1,H-1,O-16,O-16,O-16
Standard basis: CBSB7 (5D, 7F)
There are   108 symmetry adapted basis functions of A'  symmetry.
There are    36 symmetry adapted basis functions of A"  symmetry.
Crude estimate of integral set expansion from redundant integrals=1.000.
Integral buffers will be    262144 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
  144 basis functions      240 primitive gaussians
   24 alpha electrons       24 beta electrons
     nuclear repulsion energy       175.9702055832 Hartrees.
One-electron integrals computed using PRISM.
NBasis=   144 RedAO= T  NBF=   108    36
NBsUse=   144 1.00D-04 NBFU=   108    36
Initial guess read from the read-write file:
Initial guess orbital symmetries:
     Occupied  (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A') (A') (A') (A") (A")
               (A") (A') (A') (A')
     Virtual   (A") (A") (A") (A') (A') (A') (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A") (A') (A") (A') (A")
               (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
               (A') (A") (A") (A") (A') (A') (A') (A') (A") (A')
               (A") (A") (A") (A') (A") (A") (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A') (A') (A') (A") (A')
               (A') (A") (A') (A") (A") (A') (A") (A') (A") (A')
               (A") (A") (A') (A") (A') (A') (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A") (A") (A") (A') (A')
               (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
Requested convergence on RMS density matrix=1.00D-08 within  64 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Integral accuracy reduced to 1.0D-05 until final iterations.
Initial convergence to 1.0D-05 achieved.  Increase integral accuracy.
SCF Done:  E(RB+HF-LYP) =  -343.617699616     A.U. after    9 cycles
          Convg  =    0.3978D-08           -V/T =  2.0031
          S**2   =   0.0000
***** Axes restored to original set *****
---------------------------------------------------------------------
Center     Atomic                Forces (Hartrees/Bohr)
Number     Number           X             Y             Z
---------------------------------------------------------------------
   1         6        -0.000041600   -0.000071290    0.000000000
   2         1         0.000075588    0.000054068    0.000000000
   3         1         0.000002318    0.000037870    0.000000000
```

4	6	0.000016556	-0.000092201	0.000000000
5	1	0.000002445	-0.000012626	0.000000000
6	1	0.000001234	-0.000042616	0.000000000
7	6	-0.000056282	-0.000148853	0.000000000
8	1	-0.000011768	0.000019869	0.000000000
9	1	0.000022584	-0.000001865	0.000000000
10	8	0.000020747	0.000045826	0.000000000
11	8	-0.000096456	-0.000025576	0.000000000
12	8	0.000064633	0.000237393	0.000000000

Cartesian Forces: Max 0.000237393 RMS 0.000059405

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Internal Forces: Max 0.000134848 RMS 0.000026871
Search for a local minimum.
Step number 20 out of a maximum of 63
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Update second derivatives using information from points 10 11 12 13 14
15 16 17 18 19

20

Trust test= 4.47D-01 RLast= 7.25D-02 DXMaxT set to 1.00D+00
Eigenvalues --- 0.00137 0.00174 0.00230 0.01174 0.01330
Eigenvalues --- 0.01569 0.01937 0.03565 0.03565 0.05728
Eigenvalues --- 0.06546 0.07741 0.08319 0.10740 0.13315
Eigenvalues --- 0.15999 0.16734 0.17421 0.18986 0.19039
Eigenvalues --- 0.19149 0.32773 0.34455 0.35364 0.36987
Eigenvalues --- 0.37000 0.37230 0.79749 0.80442 1.03493
Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
Eigenvalues --- 1000.000001000.000001000.00000
RFO step: Lambda=-1.53790675D-07.
Quartic linear search produced a step of -0.26470.
Iteration 1 RMS(Cart)= 0.00249717 RMS(Int)= 0.00000331
Iteration 2 RMS(Cart)= 0.00000286 RMS(Int)= 0.00000191
Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000191

Variable	Old X	-DE/DX (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.09317	0.00001	0.00004	-0.00010	-0.00005	2.09312
R2	2.09318	0.00000	0.00011	-0.00008	0.00003	2.09320
R3	2.27212	0.00005	0.00002	0.00003	0.00005	2.27217
R4	5.85474	0.00001	0.00392	0.00190	0.00583	5.86058
R5	5.03592	0.00007	-0.00226	0.00199	-0.00027	5.03565
R6	5.04307	0.00002	0.01002	0.00209	0.01211	5.05518
R7	2.09053	0.00000	-0.00002	-0.00003	-0.00005	2.09048
R8	2.09074	-0.00001	0.00002	-0.00001	0.00001	2.09075
R9	2.27441	0.00002	-0.00001	0.00003	0.00002	2.27443
R10	5.88414	-0.00004	-0.00814	0.00035	-0.00779	5.87635
R11	5.06478	-0.00001	-0.01198	0.00069	-0.01129	5.05349
R12	5.08734	-0.00006	-0.00367	0.00022	-0.00345	5.08390
R13	2.09404	-0.00002	-0.00016	0.00010	-0.00006	2.09397
R14	2.09406	-0.00002	-0.00016	0.00011	-0.00006	2.09400
R15	2.27100	0.00013	0.00020	-0.00009	0.00011	2.27111
A1	1.99805	0.00003	0.00020	0.00023	0.00044	1.99849
A2	2.14259	-0.00002	-0.00005	-0.00013	-0.00018	2.14241
A3	2.14254	-0.00001	-0.00016	-0.00010	-0.00026	2.14229
A4	3.13987	0.00001	-0.00295	-0.00004	-0.00299	3.13687
A5	2.00634	0.00001	-0.00020	0.00012	-0.00007	2.00626
A6	2.13789	0.00001	0.00017	-0.00007	0.00010	2.13799
A7	2.13896	-0.00002	0.00003	-0.00005	-0.00003	2.13893
A8	2.02222	0.00000	0.00017	-0.00010	0.00006	2.02228
A9	2.13018	0.00000	-0.00008	0.00005	-0.00003	2.13016
A10	2.13079	0.00000	-0.00009	0.00005	-0.00004	2.13075
A11	2.99146	0.00002	-0.00093	0.00006	-0.00086	2.99060
A12	0.71362	0.00000	-0.00052	-0.00028	-0.00078	0.71284
A13	2.93507	-0.00003	0.00146	0.00008	0.00153	2.93660
A14	2.63450	0.00002	-0.00094	0.00020	-0.00075	2.63375
A15	0.70931	0.00001	0.00109	-0.00004	0.00104	0.71035
A16	2.85854	-0.00003	0.00082	-0.00004	0.00078	2.85931
A17	2.71534	0.00002	-0.00190	0.00009	-0.00182	2.71352
A18	3.14766	-0.00003	0.00196	-0.00011	0.00186	3.14951

A19	3.07050	0.00002	-0.00118	0.00006	-0.00112	3.06937
A20	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
A21	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D1	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D2	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D4	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D5	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D6	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D7	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D8	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D9	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D10	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D11	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D12	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D13	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D14	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D15	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D16	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D17	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

Item	Value	Threshold	Converged?
Maximum Force	0.000135	0.000450	YES
RMS Force	0.000027	0.000300	YES
Maximum Displacement	0.008005	0.001800	NO
RMS Displacement	0.002497	0.001200	NO

Predicted change in Energy=-3.521959D-07
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.564484	3.428117	0.000000
2	1	0	2.228942	2.541923	0.000000
3	1	0	0.482470	3.191070	0.000000
4	6	0	-0.081375	-0.539005	0.000000
5	1	0	0.450446	-1.509016	0.000000
6	1	0	-1.185339	-0.612019	0.000000
7	6	0	-2.201157	-4.290756	0.000000
8	1	0	-1.724129	-5.290902	0.000000
9	1	0	-3.309233	-4.283624	0.000000
10	8	0	1.983342	4.555184	0.000000
11	8	0	0.497858	0.516027	0.000000
12	8	0	-1.556272	-3.276608	0.000000

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	H	1.107630	0.000000			
3	H	1.107676	1.863212	0.000000		
4	C	4.294986	3.850933	3.772450	0.000000	
5	H	5.061261	4.424156	4.700195	1.106235	0.000000
6	H	4.887149	4.648082	4.152719	1.106375	1.865581
7	C	8.588426	8.143175	7.948559	4.309190	3.843056
8	H	9.318598	8.773820	8.764299	5.027839	4.362503
9	H	9.122723	8.789737	8.381412	4.943808	4.672647
10	O	1.202382	2.028186	2.028158	5.496710	6.254941
11	O	3.101284	2.664753	2.675088	1.203579	2.025597
12	O	7.395435	6.941408	6.781396	3.109629	2.674191

		6	7	8	9	10
6	H	0.000000				
7	C	3.816411	0.000000			
8	H	4.709803	1.108083	0.000000		
9	H	4.241652	1.108099	1.878075	0.000000	
10	O	6.061397	9.785740	10.520967	10.302227	0.000000
11	O	2.026238	5.512699	6.217527	6.126221	4.303656
12	O	2.690283	1.201821	2.021276	2.021621	8.594523

		11	12
11	O	0.000000	
12	O	4.313181	0.000000

Stoichiometry C3H6O3
Framework group CS[SG(C3H6O3)]
Deg. of freedom 21

Full point group CS NOp 2
Largest Abelian subgroup CS NOp 2
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.029422	-3.624897	0.000000
2	1	0	-1.819803	-2.848919	0.000000
3	1	0	0.004532	-3.227549	0.000000
4	6	0	0.000000	0.544898	0.000000
5	1	0	-0.671885	1.423719	0.000000
6	1	0	1.080364	0.783394	0.000000
7	6	0	1.530381	4.573180	0.000000
8	1	0	0.908123	5.490046	0.000000
9	1	0	2.626885	4.733062	0.000000
10	8	0	-1.273705	-4.802203	0.000000
11	8	0	-0.413681	-0.585354	0.000000
12	8	0	1.045639	3.473453	0.000000

Rotational constants (GHZ): 70.1259093 0.4410420 0.4382855
Isotopes: C-12,H-1,H-1,C-12,H-1,H-1,C-12,H-1,H-1,O-16,O-16,O-16
Standard basis: CBSB7 (5D, 7F)
There are 108 symmetry adapted basis functions of A' symmetry.
There are 36 symmetry adapted basis functions of A" symmetry.
Crude estimate of integral set expansion from redundant integrals=1.000.
Integral buffers will be 262144 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
144 basis functions 240 primitive gaussians
24 alpha electrons 24 beta electrons
nuclear repulsion energy 175.9786698479 Hartrees.
One-electron integrals computed using PRISM.
NBasis= 144 RedAO= T NBF= 108 36
NBsUse= 144 1.00D-04 NBFU= 108 36
Initial guess read from the read-write file:
Initial guess orbital symmetries:
Occupied (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
(A') (A') (A') (A') (A') (A') (A') (A') (A") (A")
(A") (A') (A') (A')
Virtual (A") (A") (A") (A') (A') (A') (A') (A') (A') (A')
(A') (A') (A') (A') (A') (A") (A') (A") (A') (A")
(A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
(A') (A") (A") (A") (A') (A') (A') (A') (A") (A')
(A") (A") (A") (A') (A") (A") (A') (A') (A') (A')
(A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
(A") (A") (A") (A") (A") (A") (A') (A') (A') (A')
(A') (A') (A') (A') (A') (A') (A') (A') (A') (A")
(A') (A") (A') (A") (A") (A') (A") (A') (A") (A')
(A") (A") (A') (A") (A') (A') (A') (A') (A') (A')
(A') (A') (A') (A') (A') (A") (A") (A") (A') (A')
(A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
Requested convergence on RMS density matrix=1.00D-08 within 64 cycles.
Requested convergence on MAX density matrix=1.00D-06.
SCF Done: E(RB+HF-LYP) = -343.617699995 A.U. after 8 cycles
Convg = 0.2805D-08 -V/T = 2.0031
S**2 = 0.0000
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000007531	-0.000017640	0.000000000
2	1	0.000045354	0.000032947	0.000000000
3	1	0.000000458	-0.000000236	0.000000000
4	6	0.000038155	-0.000059757	0.000000000
5	1	0.000006948	-0.000005672	0.000000000
6	1	0.000001153	-0.000040553	0.000000000
7	6	-0.000004024	-0.000068192	0.000000000
8	1	-0.000007189	0.000008664	0.000000000
9	1	0.000011424	-0.000002815	0.000000000
10	8	-0.000001366	0.000022747	0.000000000
11	8	-0.000098710	-0.000009217	0.000000000

```
 12        8        0.000000266   0.000139725   0.000000000
---------------------------------------------------------------------
Cartesian Forces:  Max     0.000139725 RMS     0.000035381

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Internal  Forces:  Max     0.000052527 RMS     0.000016567
Search for a local minimum.
Step number  21 out of a maximum of  63
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Update second derivatives using information from points 10 11 12 13 14
                                    15 16 17 18 19

                                    20 21
Trust test= 1.08D+00 RLast= 2.01D-02 DXMaxT set to 1.00D+00
   Eigenvalues ---    0.00140   0.00179   0.00230   0.01174   0.01331
   Eigenvalues ---    0.01570   0.01931   0.03565   0.03565   0.05410
   Eigenvalues ---    0.05727   0.07748   0.08211   0.09514   0.13261
   Eigenvalues ---    0.15998   0.16503   0.16951   0.18928   0.18990
   Eigenvalues ---    0.19097   0.33051   0.34458   0.35310   0.36982
   Eigenvalues ---    0.37000   0.37230   0.79779   0.80407   1.03632
   Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
   Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
   Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
   Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
   Eigenvalues --- 1000.000001000.000001000.00000
RFO step:  Lambda=-1.41653723D-07.
Quartic linear search produced a step of  0.05140.
Iteration  1 RMS(Cart)=  0.00019058 RMS(Int)=  0.00000004
Iteration  2 RMS(Cart)=  0.00000002 RMS(Int)=  0.00000003
Variable      Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                        (Linear)    (Quad)   (Total)
   R1       2.09312   0.00001   0.00000  -0.00001  -0.00001   2.09310
   R2       2.09320   0.00000   0.00000  -0.00003  -0.00002   2.09318
   R3       2.27217   0.00002   0.00000   0.00002   0.00002   2.27220
   R4       5.86058   0.00001   0.00030   0.00015   0.00045   5.86102
   R5       5.03565   0.00005  -0.00001   0.00090   0.00089   5.03654
   R6       5.05518  -0.00001   0.00062  -0.00038   0.00024   5.05543
   R7       2.09048   0.00000   0.00000   0.00000   0.00000   2.09048
   R8       2.09075   0.00000   0.00000  -0.00001  -0.00001   2.09074
   R9       2.27443   0.00000   0.00000   0.00001   0.00001   2.27444
  R10       5.87635  -0.00003  -0.00040   0.00001  -0.00039   5.87595
  R11       5.05349   0.00001  -0.00058   0.00081   0.00023   5.05372
  R12       5.08390  -0.00005  -0.00018  -0.00073  -0.00090   5.08299
  R13       2.09397  -0.00001   0.00000   0.00002   0.00001   2.09399
  R14       2.09400  -0.00001   0.00000   0.00002   0.00001   2.09402
  R15       2.27111   0.00005   0.00001   0.00000   0.00001   2.27112
   A1       1.99849   0.00001   0.00002   0.00012   0.00014   1.99863
   A2       2.14241   0.00000  -0.00001  -0.00009  -0.00009   2.14231
   A3       2.14229  -0.00001  -0.00001  -0.00003  -0.00005   2.14224
   A4       3.13687   0.00002  -0.00015   0.00029   0.00013   3.13701
   A5       2.00626   0.00000   0.00000   0.00003   0.00003   2.00629
   A6       2.13799   0.00001   0.00001  -0.00003  -0.00002   2.13797
   A7       2.13893  -0.00001   0.00000  -0.00001  -0.00001   2.13892
   A8       2.02228   0.00000   0.00000  -0.00003  -0.00003   2.02225
   A9       2.13016   0.00000   0.00000   0.00002   0.00002   2.13017
  A10       2.13075   0.00000   0.00000   0.00002   0.00002   2.13077
  A11       2.99060   0.00002  -0.00004   0.00021   0.00016   2.99077
  A12       0.71284   0.00000  -0.00004  -0.00002  -0.00006   0.71278
  A13       2.93660  -0.00003   0.00008  -0.00023  -0.00015   2.93644
  A14       2.63375   0.00002  -0.00004   0.00025   0.00021   2.63396
  A15       0.71035   0.00000   0.00005   0.00000   0.00006   0.71041
  A16       2.85931  -0.00003   0.00004  -0.00026  -0.00022   2.85910
  A17       2.71352   0.00002  -0.00009   0.00025   0.00016   2.71368
  A18       3.14951  -0.00003   0.00010  -0.00037  -0.00027   3.14924
  A19       3.06937   0.00002  -0.00006   0.00022   0.00016   3.06953
  A20       3.14159   0.00000   0.00000   0.00000   0.00000   3.14159
  A21       3.14159   0.00000   0.00000   0.00000   0.00000   3.14159
   D1       3.14159   0.00000   0.00000   0.00000   0.00000   3.14159
   D2       3.14159   0.00000   0.00000   0.00000   0.00000   3.14159
   D3       0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
   D4       3.14159   0.00000   0.00000   0.00000   0.00000   3.14159
   D5       0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
   D6       3.14159   0.00000   0.00000   0.00000   0.00000   3.14159
```

D7	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D8	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D9	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D10	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D11	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D12	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D13	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D14	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D15	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D16	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D17	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

Item	Value	Threshold	Converged?
Maximum Force	0.000053	0.000450	YES
RMS Force	0.000017	0.000300	YES
Maximum Displacement	0.000732	0.001800	YES
RMS Displacement	0.000191	0.001200	YES

Predicted change in Energy=-7.161393D-08
Optimization completed.
-- Stationary point found.

! Optimized Parameters !
! (Angstroms and Degrees) !

Name	Definition	Value	Derivative Info.
R1	R(1,2)	1.1076	-DE/DX = 0.
R2	R(1,3)	1.1077	-DE/DX = 0.
R3	R(1,10)	1.2024	-DE/DX = 0.
R4	R(1,11)	3.1013	-DE/DX = 0.
R5	R(2,11)	2.6648	-DE/DX = 0.0001
R6	R(3,11)	2.6751	-DE/DX = 0.
R7	R(4,5)	1.1062	-DE/DX = 0.
R8	R(4,6)	1.1064	-DE/DX = 0.
R9	R(4,11)	1.2036	-DE/DX = 0.
R10	R(4,12)	3.1096	-DE/DX = 0.
R11	R(5,12)	2.6742	-DE/DX = 0.
R12	R(6,12)	2.6903	-DE/DX = 0.
R13	R(7,8)	1.1081	-DE/DX = 0.
R14	R(7,9)	1.1081	-DE/DX = 0.
R15	R(7,12)	1.2018	-DE/DX = 0.0001
A1	A(2,1,3)	114.5051	-DE/DX = 0.
A2	A(2,1,10)	122.751	-DE/DX = 0.
A3	A(3,1,10)	122.7439	-DE/DX = 0.
A4	A(10,1,11)	179.7297	-DE/DX = 0.
A5	A(5,4,6)	114.9504	-DE/DX = 0.
A6	A(5,4,11)	122.498	-DE/DX = 0.
A7	A(6,4,11)	122.5516	-DE/DX = 0.
A8	A(8,7,9)	115.868	-DE/DX = 0.
A9	A(8,7,12)	122.049	-DE/DX = 0.
A10	A(9,7,12)	122.083	-DE/DX = 0.
A11	A(1,11,4)	171.3488	-DE/DX = 0.
A12	A(2,11,3)	40.8428	-DE/DX = 0.
A13	A(2,11,4)	168.2545	-DE/DX = 0.
A14	A(3,11,4)	150.9027	-DE/DX = 0.
A15	A(5,12,6)	40.7001	-DE/DX = 0.
A16	A(5,12,7)	163.8266	-DE/DX = 0.
A17	A(6,12,7)	155.4733	-DE/DX = 0.
A18	L(11,4,12,3,-1)	180.4539	-DE/DX = 0.
A19	L(4,12,7,9,-1)	175.862	-DE/DX = 0.
A20	L(11,4,12,3,-2)	180.	-DE/DX = 0.
A21	L(4,12,7,9,-2)	180.	-DE/DX = 0.
D1	D(10,1,11,4)	180.	-DE/DX = 0.
D2	D(5,4,11,1)	180.	-DE/DX = 0.
D3	D(5,4,11,2)	0.	-DE/DX = 0.
D4	D(5,4,11,3)	180.	-DE/DX = 0.
D5	D(6,4,11,1)	0.	-DE/DX = 0.
D6	D(6,4,11,2)	180.	-DE/DX = 0.
D7	D(6,4,11,3)	0.	-DE/DX = 0.
D8	D(8,7,11,1)	180.	-DE/DX = 0.
D9	D(8,7,11,2)	0.	-DE/DX = 0.
D10	D(8,7,11,3)	180.	-DE/DX = 0.
D11	D(9,7,11,1)	0.	-DE/DX = 0.
D12	D(9,7,11,2)	180.	-DE/DX = 0.
D13	D(9,7,11,3)	0.	-DE/DX = 0.

```
! D14   D(8,7,12,5)          0.          -DE/DX =    0.           !
! D15   D(8,7,12,6)        180.          -DE/DX =    0.           !
! D16   D(9,7,12,5)        180.          -DE/DX =    0.           !
! D17   D(9,7,12,6)          0.          -DE/DX =    0.           !
---------------------------------------------------------------------------
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

                     Input orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic          Coordinates (Angstroms)
Number     Number      Type             X           Y           Z
---------------------------------------------------------------------
     1          6           0        1.563770    3.428442    0.000000
     2          1           0        2.228228    2.542248    0.000000
     3          1           0        0.481755    3.191396    0.000000
     4          6           0       -0.082090   -0.538679    0.000000
     5          1           0        0.449731   -1.508691    0.000000
     6          1           0       -1.186053   -0.611694    0.000000
     7          6           0       -2.201872   -4.290431    0.000000
     8          1           0       -1.724843   -5.290577    0.000000
     9          1           0       -3.309947   -4.283299    0.000000
    10          8           0        1.982628    4.555509    0.000000
    11          8           0        0.497144    0.516352    0.000000
    12          8           0       -1.556987   -3.276282    0.000000
---------------------------------------------------------------------
               Distance matrix (angstroms):
                     1          2          3          4          5
     1  C    0.000000
     2  H    1.107630   0.000000
     3  H    1.107676   1.863212   0.000000
     4  C    4.294986   3.850933   3.772450   0.000000
     5  H    5.061261   4.424156   4.700195   1.106235   0.000000
     6  H    4.887149   4.648082   4.152719   1.106375   1.865581
     7  C    8.588426   8.143175   7.948559   4.309190   3.843056
     8  H    9.318598   8.773820   8.764299   5.027839   4.362503
     9  H    9.122723   8.789737   8.381412   4.943808   4.672647
    10  O    1.202382   2.028186   2.028158   5.496710   6.254941
    11  O    3.101284   2.664753   2.675088   1.203579   2.025597
    12  O    7.395435   6.941408   6.781396   3.109629   2.674191
                    6          7          8          9         10
     6  H    0.000000
     7  C    3.816411   0.000000
     8  H    4.709803   1.108083   0.000000
     9  H    4.241652   1.108099   1.878075   0.000000
    10  O    6.061397   9.785740  10.520967  10.302227   0.000000
    11  O    2.026238   5.512699   6.217527   6.126221   4.303656
    12  O    2.690283   1.201821   2.021276   2.021621   8.594523
                   11         12
    11  O    0.000000
    12  O    4.313181   0.000000
Stoichiometry    C3H6O3
Framework group  CS[SG(C3H6O3)]
Deg. of freedom   21
Full point group                 CS     NOp   2
Largest Abelian subgroup         CS     NOp   2
Largest concise Abelian subgroup C1     NOp   1
                    Standard orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic          Coordinates (Angstroms)
Number     Number      Type             X           Y           Z
---------------------------------------------------------------------
     1          6           0       -1.029422   -3.624897    0.000000
     2          1           0       -1.819803   -2.848919    0.000000
     3          1           0        0.004532   -3.227549    0.000000
     4          6           0        0.000000    0.544898    0.000000
     5          1           0       -0.671885    1.423719    0.000000
     6          1           0        1.080364    0.783394    0.000000
     7          6           0        1.530381    4.573180    0.000000
     8          1           0        0.908123    5.490046    0.000000
     9          1           0        2.626885    4.733062    0.000000
    10          8           0       -1.273705   -4.802203    0.000000
    11          8           0       -0.413681   -0.585354    0.000000
    12          8           0        1.045639    3.473453    0.000000
---------------------------------------------------------------------
```

Rotational constants (GHZ): 70.1259093 0.4410420 0.4382855
Isotopes: C-12,H-1,H-1,C-12,H-1,H-1,C-12,H-1,H-1,O-16,O-16,O-16

****

Population analysis using the SCF density.

****

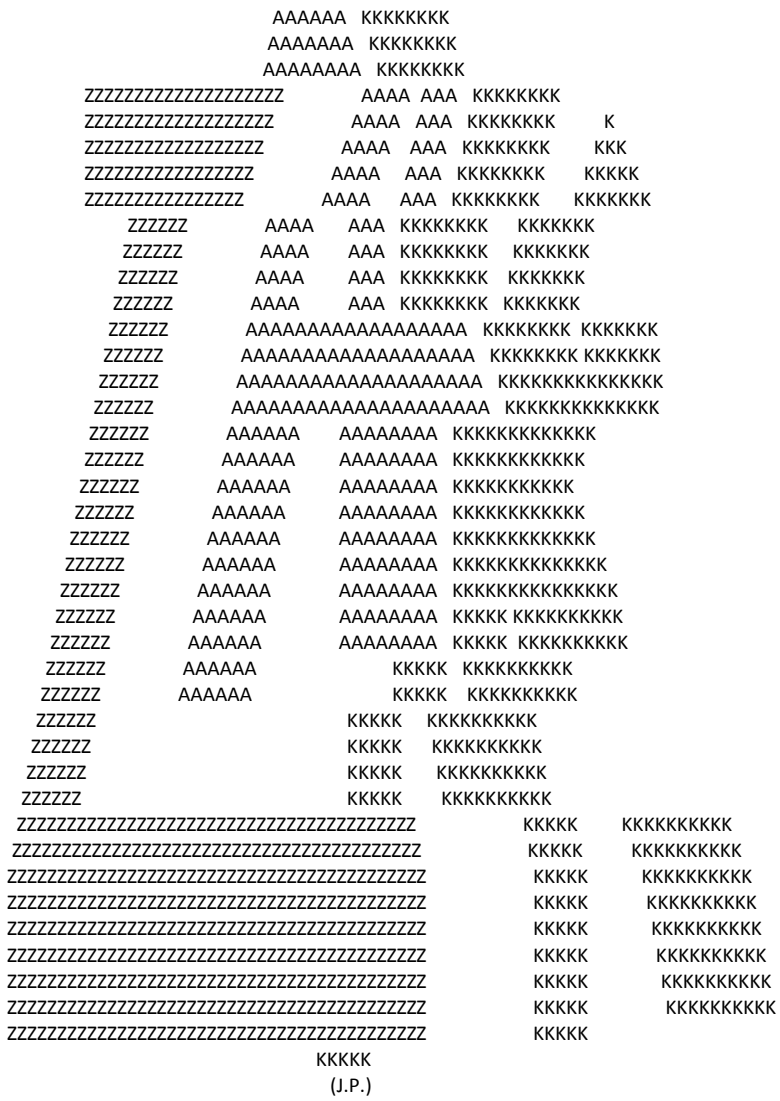
Orbital Symmetries:
Occupied (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
(A') (A') (A') (A') (A') (A') (A') (A') (A") (A")
(A") (A') (A') (A')
Virtual (A") (A") (A") (A') (A') (A') (A') (A') (A') (A')
(A') (A') (A') (A') (A') (A") (A') (A") (A') (A")
(A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
(A') (A") (A") (A") (A') (A') (A') (A') (A") (A')
(A") (A") (A") (A') (A") (A") (A') (A') (A') (A')
(A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
(A") (A") (A") (A") (A") (A") (A') (A') (A') (A')
(A') (A') (A') (A') (A') (A') (A') (A') (A') (A")
(A') (A") (A') (A") (A") (A') (A") (A') (A") (A')
(A") (A") (A') (A") (A') (A') (A') (A') (A') (A')
(A') (A') (A') (A') (A') (A") (A") (A") (A') (A')
(A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
The electronic state is 1-A'.
Alpha occ. eigenvalues -- -19.16023 -19.13632 -19.11234 -10.29158 -10.26528
Alpha occ. eigenvalues -- -10.24312 -1.08980 -1.06528 -1.04279 -0.65882
Alpha occ. eigenvalues -- -0.63297 -0.61034 -0.52038 -0.49414 -0.48245
Alpha occ. eigenvalues -- -0.47218 -0.45628 -0.42984 -0.42813 -0.40443
Alpha occ. eigenvalues -- -0.38213 -0.29582 -0.27083 -0.24658
Alpha virt. eigenvalues -- -0.07068 -0.04630 -0.02366 0.03377 0.06373
Alpha virt. eigenvalues -- 0.08480 0.08575 0.11524 0.14446 0.16519
Alpha virt. eigenvalues -- 0.20061 0.24182 0.29535 0.34201 0.36239
Alpha virt. eigenvalues -- 0.36464 0.37725 0.38830 0.39757 0.40977
Alpha virt. eigenvalues -- 0.41719 0.50820 0.54526 0.55884 0.57967
Alpha virt. eigenvalues -- 0.58837 0.61145 0.63894 0.65561 0.67324
Alpha virt. eigenvalues -- 0.76317 0.79626 0.83183 0.86865 0.88708
Alpha virt. eigenvalues -- 0.89820 0.92279 0.93944 0.98721 0.99028
Alpha virt. eigenvalues -- 1.01495 1.03574 1.23584 1.25900 1.25956
Alpha virt. eigenvalues -- 1.27923 1.32523 1.36608 1.37104 1.37607
Alpha virt. eigenvalues -- 1.40436 1.42866 1.46781 1.48837 1.55779
Alpha virt. eigenvalues -- 1.58995 1.59067 1.60869 1.61908 1.64083
Alpha virt. eigenvalues -- 1.71649 1.74893 1.77081 1.82017 1.84370
Alpha virt. eigenvalues -- 1.86102 2.05486 2.10529 2.13043 2.26177
Alpha virt. eigenvalues -- 2.28812 2.31349 2.38089 2.40288 2.41993
Alpha virt. eigenvalues -- 2.43039 2.43840 2.44840 2.51253 2.54021
Alpha virt. eigenvalues -- 2.55216 2.56822 2.56886 2.59026 2.84608
Alpha virt. eigenvalues -- 2.86220 2.86853 2.88847 2.89209 2.91109
Alpha virt. eigenvalues -- 3.28032 3.30241 3.31950 3.32741 3.34935
Alpha virt. eigenvalues -- 3.37178 3.41244 3.42958 3.44548 3.66863
Alpha virt. eigenvalues -- 3.70410 3.72536 3.79868 3.85448 3.88195
Alpha virt. eigenvalues -- 4.79393 4.82445 4.85497 4.93015 4.95833
Alpha virt. eigenvalues -- 4.99948 5.51585 5.52884 5.55410 23.82789
Alpha virt. eigenvalues -- 23.86055 23.88356 49.86903 49.90305 49.92835
Condensed to atoms (all electrons):

		1	2	3	4	5	6
1	C	4.602840	0.368220	0.364720	0.000020	0.000042	0.000065
2	H	0.368220	0.696899	-0.099827	-0.000393	-0.000444	0.000365
3	H	0.364720	-0.099827	0.702073	-0.000429	0.000391	-0.000813
4	C	0.000020	-0.000393	-0.000429	4.610107	0.368206	0.366397
5	H	0.000042	-0.000444	0.000391	0.368206	0.682380	-0.095065
6	H	0.000065	0.000365	-0.000813	0.366397	-0.095065	0.687562
7	C	0.000000	0.000000	0.000000	0.000024	-0.000421	-0.000413
8	H	0.000000	0.000000	0.000000	0.000049	-0.000515	0.000370
9	H	0.000000	0.000000	0.000000	0.000052	0.000370	-0.000670
10	O	0.574110	-0.052912	-0.052349	-0.000003	0.000000	0.000000
11	O	-0.002736	0.009044	0.011434	0.557872	-0.049997	-0.050954
12	O	0.000000	0.000000	0.000000	-0.002507	0.009380	0.010265

		7	8	9	10	11	12
1	C	0.000000	0.000000	0.000000	0.574110	-0.002736	0.000000
2	H	0.000000	0.000000	0.000000	-0.052912	0.009044	0.000000
3	H	0.000000	0.000000	0.000000	-0.052349	0.011434	0.000000
4	C	0.000024	0.000049	0.000052	-0.000003	0.557872	-0.002507

```
 5  H   -0.000421  -0.000515   0.000370   0.000000  -0.049997   0.009380
 6  H   -0.000413   0.000370  -0.000670   0.000000  -0.050954   0.010265
 7  C    4.588219   0.366791   0.366626   0.000000  -0.000003   0.571831
 8  H    0.366791   0.692024  -0.093948   0.000000   0.000000  -0.051094
 9  H    0.366626  -0.093948   0.693069   0.000000   0.000000  -0.051572
10  O    0.000000   0.000000   0.000000   7.802425   0.000059   0.000000
11  O   -0.000003   0.000000   0.000000   0.000059   7.793262   0.000057
12  O    0.571831  -0.051094  -0.051572   0.000000   0.000057   7.769752
Total atomic charges:
          1
 1  C    0.092720
 2  H    0.079048
 3  H    0.074800
 4  C    0.100608
 5  H    0.085671
 6  H    0.082891
 7  C    0.107345
 8  H    0.086322
 9  H    0.086073
10  O   -0.271330
11  O   -0.268037
12  O   -0.256111
Sum of Mulliken charges=   0.00000
Atomic charges with hydrogens summed into heavy atoms:
          1
 1  C    0.246569
 2  H    0.000000
 3  H    0.000000
 4  C    0.269170
 5  H    0.000000
 6  H    0.000000
 7  C    0.279740
 8  H    0.000000
 9  H    0.000000
10  O   -0.271330
11  O   -0.268037
12  O   -0.256111
Sum of Mulliken charges=   0.00000
Electronic spatial extent (au):  <R**2>=  2291.3026
Charge=     0.0000 electrons
Dipole moment (Debye):
   X=     2.4598    Y=     7.4836    Z=     0.0000  Tot=     7.8775
Quadrupole moment (Debye-Ang):
  XX=   -33.6355   YY=   -36.9664   ZZ=   -34.5839
  XY=     1.4907   XZ=     0.0000   YZ=     0.0000
Octapole moment (Debye-Ang**2):
 XXX=     8.2293  YYY=   242.5336  ZZZ=     0.0000  XYY=    71.7935
 XXY=    23.3380  XXZ=     0.0000  XZZ=    -0.6976  YZZ=    -2.0116
 YYZ=     0.0000  XYZ=     0.0000
Hexadecapole moment (Debye-Ang**3):
XXXX=  -268.6415 YYYY= -2611.7081 ZZZZ=   -29.3273 XXXY=  -347.5199
XXXZ=     0.0000 YYYX=  -347.8125 YYYZ=     0.0000 ZZZX=     0.0000
ZZZY=     0.0000 XXYY=  -435.9379 XXZZ=   -51.8445 YYZZ=  -415.6558
XXYZ=     0.0000 YYXZ=     0.0000 ZZXY=  -120.4378
N-N= 1.759786698479D+02 E-N=-1.159673891669D+03  KE= 3.425627336963D+02
Symmetry A'   KE= 3.314630982715D+02
Symmetry A"   KE= 1.109963542487D+01
1|1|UNPC-UNK|FOpt|RB3LYP|CBSB7|C3H6O3|PCUSER|11-Oct-2015|0||# OPT FREQ
 CBS-QB3 6-311++G(D,P) GEOM=CONNECTIVITY||Title Card Required||0,1|C,1
.5637698791,3.4284420444,0.|H,2.2282278702,2.5422482383,0.|H,0.4817554
76,3.1913956349,0.|C,-0.0820898157,-0.5386793693,0.|H,0.4497309692,-1.
5086906652,0.|H,-1.1860533013,-0.6116939792,0.|C,-2.2018717885,-4.2904
312843,0.|H,-1.7248430438,-5.2905769429,0.|H,-3.3099473356,-4.28329886
36,0.|O,1.9826278561,4.5555092219,0.|O,0.4971437781,0.5163517725,0.|O,
-1.5569866697,-3.2762824654,0.||Version=x86-Win32-G98RevA.11.4|State=1
-A'|HF=-343.6177|RMSD=2.805e-009|RMSF=3.538e-005|Dipole=-1.4002579,-2.
7648661,0.|PG=CS [SG(C3H6O3)]||@
```

A
AA
AAA
AAAA
AAAAA



(J.P.)

Job cpu time: 0 days 0 hours 18 minutes 44.0 seconds.
File lengths (MBytes): RWF=   15 Int=   0 D2E=   0 Chk=   5 Scr=   1
Normal termination of Gaussian 98.
Link1: Proceeding to internal job step number 2.

#N Geom=AllCheck Guess=TCheck B3LYP/CBSB7 Freq

1/10=4,29=7,30=1,38=1/1,3;
2/40=1/2;
3/5=4,6=6,7=700,11=2,25=1,30=1/1,2,3;
4/5=101/1;
5/5=2,42=-5/2;
8/6=4,11=11,23=2,27=262144000/1;
11/6=1,8=1,9=11,15=111,16=11/1,2,10;
10/6=1/2;
6/7=2,8=2,9=2,10=2,18=1,28=1/1;
7/8=1,10=1,25=1/1,2,3,16;
1/10=4,30=1/3;
99//99;

Title Card Required

Redundant internal coordinates taken from checkpoint file:
C:\Users\hp\Desktop\3_cbsqb3.chk
Charge = 0 Multiplicity = 1
C,0,1.5637698791,3.4284420444,0.
H,0,2.2282278702,2.5422482383,0.
H,0,0.481755476,3.1913956349,0.
C,0,-0.0820898157,-0.5386793693,0.
H,0,0.4497309692,-1.5086906652,0.
H,0,-1.1860533013,-0.6116939792,0.
C,0,-2.2018717885,-4.2904312843,0.

H,0,-1.7248430438,-5.2905769429,0.
H,0,-3.3099473356,-4.2832988636,0.
O,0,1.9826278561,4.5555092219,0.
O,0,0.4971437781,0.5163517725,0.
O,0,-1.5569866697,-3.2762824654,0.
Recover connectivity data from disk.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Initialization pass.

! Initial Parameters !
! (Angstroms and Degrees) !

Name	Definition	Value	Derivative Info.
R1	R(1,2)	1.1076	calculate D2E/DX2 analytically!
R2	R(1,3)	1.1077	calculate D2E/DX2 analytically!
R3	R(1,10)	1.2024	calculate D2E/DX2 analytically!
R4	R(1,11)	3.1013	calculate D2E/DX2 analytically!
R5	R(2,11)	2.6648	calculate D2E/DX2 analytically!
R6	R(3,11)	2.6751	calculate D2E/DX2 analytically!
R7	R(4,5)	1.1062	calculate D2E/DX2 analytically!
R8	R(4,6)	1.1064	calculate D2E/DX2 analytically!
R9	R(4,11)	1.2036	calculate D2E/DX2 analytically!
R10	R(4,12)	3.1096	calculate D2E/DX2 analytically!
R11	R(5,12)	2.6742	calculate D2E/DX2 analytically!
R12	R(6,12)	2.6903	calculate D2E/DX2 analytically!
R13	R(7,8)	1.1081	calculate D2E/DX2 analytically!
R14	R(7,9)	1.1081	calculate D2E/DX2 analytically!
R15	R(7,12)	1.2018	calculate D2E/DX2 analytically!
A1	A(2,1,3)	114.5051	calculate D2E/DX2 analytically!
A2	A(2,1,10)	122.751	calculate D2E/DX2 analytically!
A3	A(3,1,10)	122.7439	calculate D2E/DX2 analytically!
A4	A(10,1,11)	179.7297	calculate D2E/DX2 analytically!
A5	A(5,4,6)	114.9504	calculate D2E/DX2 analytically!
A6	A(5,4,11)	122.498	calculate D2E/DX2 analytically!
A7	A(6,4,11)	122.5516	calculate D2E/DX2 analytically!
A8	A(8,7,9)	115.868	calculate D2E/DX2 analytically!
A9	A(8,7,12)	122.049	calculate D2E/DX2 analytically!
A10	A(9,7,12)	122.083	calculate D2E/DX2 analytically!
A11	A(1,11,4)	171.3488	calculate D2E/DX2 analytically!
A12	A(2,11,3)	40.8428	calculate D2E/DX2 analytically!
A13	A(2,11,4)	168.2545	calculate D2E/DX2 analytically!
A14	A(3,11,4)	150.9027	calculate D2E/DX2 analytically!
A15	A(5,12,6)	40.7001	calculate D2E/DX2 analytically!
A16	A(5,12,7)	163.8266	calculate D2E/DX2 analytically!
A17	A(6,12,7)	155.4733	calculate D2E/DX2 analytically!
A18	L(11,4,12,3,-1)	180.4539	calculate D2E/DX2 analytically!
A19	L(4,12,7,9,-1)	175.862	calculate D2E/DX2 analytically!
A20	L(11,4,12,3,-2)	180.	calculate D2E/DX2 analytically!
A21	L(4,12,7,9,-2)	180.	calculate D2E/DX2 analytically!
D1	D(10,1,11,4)	180.	calculate D2E/DX2 analytically!
D2	D(5,4,11,1)	180.	calculate D2E/DX2 analytically!
D3	D(5,4,11,2)	0.	calculate D2E/DX2 analytically!
D4	D(5,4,11,3)	180.	calculate D2E/DX2 analytically!
D5	D(6,4,11,1)	0.	calculate D2E/DX2 analytically!
D6	D(6,4,11,2)	180.	calculate D2E/DX2 analytically!
D7	D(6,4,11,3)	0.	calculate D2E/DX2 analytically!
D8	D(8,7,11,1)	180.	calculate D2E/DX2 analytically!
D9	D(8,7,11,2)	0.	calculate D2E/DX2 analytically!
D10	D(8,7,11,3)	180.	calculate D2E/DX2 analytically!
D11	D(9,7,11,1)	0.	calculate D2E/DX2 analytically!
D12	D(9,7,11,2)	180.	calculate D2E/DX2 analytically!
D13	D(9,7,11,3)	0.	calculate D2E/DX2 analytically!
D14	D(8,7,12,5)	0.	calculate D2E/DX2 analytically!
D15	D(8,7,12,6)	180.	calculate D2E/DX2 analytically!
D16	D(9,7,12,5)	180.	calculate D2E/DX2 analytically!
D17	D(9,7,12,6)	0.	calculate D2E/DX2 analytically!

Trust Radius=3.00D-01 FncErr=1.00D-07 GrdErr=1.00D-07
Number of steps in this run= 63 maximum allowed number of steps= 100.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.563770	3.428442	0.000000
2	1	0	2.228228	2.542248	0.000000
3	1	0	0.481755	3.191396	0.000000
4	6	0	-0.082090	-0.538679	0.000000
5	1	0	0.449731	-1.508691	0.000000
6	1	0	-1.186053	-0.611694	0.000000
7	6	0	-2.201872	-4.290431	0.000000
8	1	0	-1.724843	-5.290577	0.000000
9	1	0	-3.309947	-4.283299	0.000000
10	8	0	1.982628	4.555509	0.000000
11	8	0	0.497144	0.516352	0.000000
12	8	0	-1.556987	-3.276282	0.000000

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	H	1.107630	0.000000			
3	H	1.107676	1.863212	0.000000		
4	C	4.294986	3.850933	3.772450	0.000000	
5	H	5.061261	4.424156	4.700195	1.106235	0.000000
6	H	4.887149	4.648082	4.152719	1.106375	1.865581
7	C	8.588426	8.143175	7.948559	4.309190	3.843056
8	H	9.318598	8.773820	8.764299	5.027839	4.362503
9	H	9.122723	8.789737	8.381412	4.943808	4.672647
10	O	1.202382	2.028186	2.028158	5.496710	6.254941
11	O	3.101284	2.664753	2.675088	1.203579	2.025597
12	O	7.395435	6.941408	6.781396	3.109629	2.674191

		6	7	8	9	10
6	H	0.000000				
7	C	3.816411	0.000000			
8	H	4.709803	1.108083	0.000000		
9	H	4.241652	1.108099	1.878075	0.000000	
10	O	6.061397	9.785740	10.520967	10.302227	0.000000
11	O	2.026238	5.512699	6.217527	6.126221	4.303656
12	O	2.690283	1.201821	2.021276	2.021621	8.594523

		11	12
11	O	0.000000	
12	O	4.313181	0.000000

Interatomic angles:

H2-C1-H3=114.5051 H5-C4-H6=114.9504 H8-C7-H9=115.868
H2-C1-O10=122.751 H3-C1-O10=122.7439 H2-H3-O10= 62.6567
C1-H2-O11=102.6247 C1-H3-O11=102.0275 H3-H2-O11= 69.8765
H2-O11-C4=168.2545 H3-O11-C4=150.9027 H2-O11-H5=140.8281
H3-O11-H5=178.3292 H5-C4-O11=122.498 H2-O11-H6=164.3424
H3-O11-H6=123.4996 H6-C4-O11=122.5516 H6-H5-O11= 62.6027
O10-H2-O11=132.5316 O10-H3-O11=131.9375 C4-H5-O12=102.6405
C4-H6-O12=101.7091 H6-H5-O12= 70.1134 H5-O12-C7=163.8266
H6-O12-C7=155.4733 H5-O12-H8=136.1384 H6-O12-H8=176.8385
H8-C7-O12=122.049 H5-O12-H9=168.5011 H6-O12-H9=127.801
H9-C7-O12=122.083 H9-H8-O12= 62.3291 O11-H5-O12=132.716
O11-H6-O12=131.7543

Stoichiometry C3H6O3
Framework group CS[SG(C3H6O3)]
Deg. of freedom 21
Full point group CS NOp 2
Largest Abelian subgroup CS NOp 2
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.029422	-3.624897	0.000000
2	1	0	-1.819803	-2.848919	0.000000
3	1	0	0.004532	-3.227549	0.000000
4	6	0	0.000000	0.544898	0.000000
5	1	0	-0.671885	1.423719	0.000000
6	1	0	1.080364	0.783394	0.000000
7	6	0	1.530381	4.573180	0.000000

```
  8        1          0      0.908123    5.490046    0.000000
  9        1          0      2.626885    4.733062    0.000000
 10        8          0     -1.273705   -4.802203    0.000000
 11        8          0     -0.413681   -0.585354    0.000000
 12        8          0      1.045639    3.473453    0.000000
---------------------------------------------------------------------
Rotational constants (GHZ):     70.1259093      0.4410420      0.4382855
Isotopes: C-12,H-1,H-1,C-12,H-1,H-1,C-12,H-1,H-1,O-16,O-16,O-16
Standard basis: CBSB7 (5D, 7F)
There are   108 symmetry adapted basis functions of A'  symmetry.
There are    36 symmetry adapted basis functions of A"  symmetry.
Crude estimate of integral set expansion from redundant integrals=1.000.
Integral buffers will be    262144 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
  144 basis functions      240 primitive gaussians
   24 alpha electrons       24 beta electrons
     nuclear repulsion energy       175.9786698479 Hartrees.
One-electron integrals computed using PRISM.
NBasis=   144 RedAO= T  NBF=   108    36
NBsUse=   144 1.00D-04 NBFU=   108    36
Initial guess read from the checkpoint file:
C:\Users\hp\Desktop\3_cbsqb3.chk
Initial guess orbital symmetries:
     Occupied  (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A') (A') (A') (A") (A")
               (A") (A') (A') (A')
     Virtual   (A") (A") (A") (A') (A') (A') (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A") (A') (A") (A') (A")
               (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
               (A') (A") (A") (A") (A') (A') (A') (A') (A") (A')
               (A") (A") (A") (A') (A") (A") (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
               (A") (A") (A") (A") (A") (A") (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A') (A') (A') (A') (A")
               (A') (A") (A') (A") (A") (A') (A") (A') (A") (A')
               (A") (A") (A') (A") (A') (A') (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A") (A") (A") (A') (A')
               (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
Requested convergence on RMS density matrix=1.00D-08 within  64 cycles.
Requested convergence on MAX density matrix=1.00D-06.
SCF Done:  E(RB+HF-LYP) =  -343.617699995     A.U. after    1 cycles
          Convg  =    0.1952D-08           -V/T =  2.0031
          S**2   =   0.0000
Range of M.O.s used for correlation:     1   144
NBasis=   144 NAE=    24 NBE=    24 NFC=     0 NFV=     0
NROrb=    144 NOA=    24 NOB=    24 NVA=   120 NVB=   120
G2DrvN: will do   12 atoms at a time, making    1 passes doing MaxLOS=2.
FoFDir used for L=0 through L=2.
       Differentiating once with respect to electric field.
          with respect to dipole field.
       Differentiating once with respect to nuclear coordinates.
Integrals replicated using symmetry in FoFDir.
MinBra= 0 MaxBra= 2 Meth= 1.
IRaf=      0 NMat=  39 IRICut=      39 DoRegI=T DoRafI=T ISym2E= 2 JSym2E=2.
Raff turned off since only 65.32% of shell-pairs survive.
       There are  39 degrees of freedom in the 1st order CPHF.
 37 vectors were produced by pass  0.
AX will form  37 AO Fock derivatives at one time.
 36 vectors were produced by pass  1.
 36 vectors were produced by pass  2.
 36 vectors were produced by pass  3.
 34 vectors were produced by pass  4.
 26 vectors were produced by pass  5.
  3 vectors were produced by pass  6.
  1 vectors were produced by pass  7.
Inv2:  IOpt= 1 Iter= 1 AM= 2.45D-15 Conv= 1.00D-12.
Inverted reduced A of dimension 209 with in-core refinement.

*******************************************************************

        Population analysis using the SCF density.

*******************************************************************
```

Orbital Symmetries:
Occupied (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
(A') (A') (A') (A') (A') (A') (A') (A') (A") (A")
(A") (A') (A') (A')
Virtual (A") (A") (A") (A') (A') (A') (A') (A') (A') (A')
(A') (A') (A') (A') (A') (A") (A') (A") (A') (A")
(A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
(A') (A") (A") (A") (A') (A') (A') (A') (A") (A')
(A") (A") (A") (A') (A") (A") (A') (A') (A') (A')
(A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
(A") (A") (A") (A") (A") (A") (A') (A') (A') (A')
(A') (A') (A') (A') (A') (A') (A') (A') (A') (A")
(A') (A") (A') (A") (A") (A') (A") (A') (A") (A')
(A") (A") (A') (A") (A') (A') (A') (A') (A') (A')
(A') (A') (A') (A') (A') (A") (A") (A") (A') (A')
(A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
The electronic state is 1-A'.
Alpha occ. eigenvalues -- -19.16023 -19.13632 -19.11234 -10.29158 -10.26528
Alpha occ. eigenvalues -- -10.24312 -1.08980 -1.06528 -1.04279 -0.65882
Alpha occ. eigenvalues -- -0.63297 -0.61034 -0.52038 -0.49414 -0.48245
Alpha occ. eigenvalues -- -0.47218 -0.45628 -0.42984 -0.42813 -0.40443
Alpha occ. eigenvalues -- -0.38213 -0.29582 -0.27083 -0.24658
Alpha virt. eigenvalues -- -0.07068 -0.04630 -0.02366 0.03377 0.06373
Alpha virt. eigenvalues -- 0.08480 0.08575 0.11524 0.14446 0.16519
Alpha virt. eigenvalues -- 0.20061 0.24182 0.29535 0.34201 0.36239
Alpha virt. eigenvalues -- 0.36464 0.37725 0.38830 0.39757 0.40977
Alpha virt. eigenvalues -- 0.41719 0.50820 0.54526 0.55884 0.57967
Alpha virt. eigenvalues -- 0.58837 0.61145 0.63894 0.65561 0.67324
Alpha virt. eigenvalues -- 0.76317 0.79626 0.83183 0.86865 0.88708
Alpha virt. eigenvalues -- 0.89820 0.92279 0.93944 0.98721 0.99028
Alpha virt. eigenvalues -- 1.01495 1.03574 1.23584 1.25900 1.25956
Alpha virt. eigenvalues -- 1.27923 1.32523 1.36608 1.37104 1.37607
Alpha virt. eigenvalues -- 1.40436 1.42866 1.46781 1.48837 1.55779
Alpha virt. eigenvalues -- 1.58995 1.59067 1.60869 1.61908 1.64083
Alpha virt. eigenvalues -- 1.71649 1.74893 1.77081 1.82017 1.84370
Alpha virt. eigenvalues -- 1.86102 2.05486 2.10529 2.13043 2.26177
Alpha virt. eigenvalues -- 2.28812 2.31349 2.38089 2.40288 2.41993
Alpha virt. eigenvalues -- 2.43039 2.43840 2.44840 2.51253 2.54021
Alpha virt. eigenvalues -- 2.55216 2.56822 2.56886 2.59026 2.84608
Alpha virt. eigenvalues -- 2.86220 2.86853 2.88847 2.89209 2.91109
Alpha virt. eigenvalues -- 3.28032 3.30241 3.31950 3.32741 3.34935
Alpha virt. eigenvalues -- 3.37178 3.41244 3.42958 3.44548 3.66863
Alpha virt. eigenvalues -- 3.70410 3.72536 3.79868 3.85448 3.88195
Alpha virt. eigenvalues -- 4.79393 4.82445 4.85497 4.93015 4.95833
Alpha virt. eigenvalues -- 4.99948 5.51585 5.52884 5.55410 23.82789
Alpha virt. eigenvalues -- 23.86055 23.88356 49.86903 49.90305 49.92835
Condensed to atoms (all electrons):

		1	2	3	4	5	6
1	C	4.602840	0.368220	0.364720	0.000020	0.000042	0.000065
2	H	0.368220	0.696899	-0.099827	-0.000393	-0.000444	0.000365
3	H	0.364720	-0.099827	0.702073	-0.000429	0.000391	-0.000813
4	C	0.000020	-0.000393	-0.000429	4.610107	0.368206	0.366397
5	H	0.000042	-0.000444	0.000391	0.368206	0.682381	-0.095065
6	H	0.000065	0.000365	-0.000813	0.366397	-0.095065	0.687562
7	C	0.000000	0.000000	0.000000	0.000024	-0.000421	-0.000413
8	H	0.000000	0.000000	0.000000	0.000049	-0.000515	0.000370
9	H	0.000000	0.000000	0.000000	0.000052	0.000370	-0.000670
10	O	0.574109	-0.052912	-0.052349	-0.000003	0.000000	0.000000
11	O	-0.002736	0.009044	0.011434	0.557872	-0.049997	-0.050954
12	O	0.000000	0.000000	0.000000	-0.002507	0.009380	0.010265

		7	8	9	10	11	12
1	C	0.000000	0.000000	0.000000	0.574109	-0.002736	0.000000
2	H	0.000000	0.000000	0.000000	-0.052912	0.009044	0.000000
3	H	0.000000	0.000000	0.000000	-0.052349	0.011434	0.000000
4	C	0.000024	0.000049	0.000052	-0.000003	0.557872	-0.002507
5	H	-0.000421	-0.000515	0.000370	0.000000	-0.049997	0.009380
6	H	-0.000413	0.000370	-0.000670	0.000000	-0.050954	0.010265
7	C	4.588219	0.366791	0.366626	0.000000	-0.000003	0.571831
8	H	0.366791	0.692024	-0.093948	0.000000	0.000000	-0.051094
9	H	0.366626	-0.093948	0.693069	0.000000	0.000000	-0.051572
10	O	0.000000	0.000000	0.000000	7.802426	0.000059	0.000000
11	O	-0.000003	0.000000	0.000000	0.000059	7.793262	0.000057
12	O	0.571831	-0.051094	-0.051572	0.000000	0.000057	7.769752

Total atomic charges:

		1
1	C	0.092721
2	H	0.079048
3	H	0.074800
4	C	0.100607
5	H	0.085671
6	H	0.082891
7	C	0.107345
8	H	0.086322
9	H	0.086073
10	O	-0.271330
11	O	-0.268037
12	O	-0.256111

Sum of Mulliken charges= 0.00000
Atomic charges with hydrogens summed into heavy atoms:

		1
1	C	0.246569
2	H	0.000000
3	H	0.000000
4	C	0.269169
5	H	0.000000
6	H	0.000000
7	C	0.279740
8	H	0.000000
9	H	0.000000
10	O	-0.271330
11	O	-0.268037
12	O	-0.256111

Sum of Mulliken charges= 0.00000
Electronic spatial extent (au): <R**2>= 2291.3026
Charge= 0.0000 electrons
Dipole moment (Debye):
X= 2.4598 Y= 7.4836 Z= 0.0000 Tot= 7.8775
Quadrupole moment (Debye-Ang):
XX= -33.6355 YY= -36.9664 ZZ= -34.5839
XY= 1.4907 XZ= 0.0000 YZ= 0.0000
Octapole moment (Debye-Ang**2):
XXX= 8.2293 YYY= 242.5336 ZZZ= 0.0000 XYY= 71.7935
XXY= 23.3380 XXZ= 0.0000 XZZ= -0.6976 YZZ= -2.0116
YYZ= 0.0000 XYZ= 0.0000
Hexadecapole moment (Debye-Ang**3):
XXXX= -268.6415 YYYY= -2611.7085 ZZZZ= -29.3273 XXXY= -347.5199
XXXZ= 0.0000 YYYX= -347.8126 YYYZ= 0.0000 ZZZX= 0.0000
ZZZY= 0.0000 XXYY= -435.9379 XXZZ= -51.8445 YYZZ= -415.6558
XXYZ= 0.0000 YYXZ= 0.0000 ZZXY= -120.4378
N-N= 1.759786698479D+02 E-N=-1.159673889691D+03 KE= 3.425627328030D+02
Symmetry A' KE= 3.314630977529D+02
Symmetry A" KE= 1.109963505005D+01
Exact polarizability: 43.841 7.726 65.272 0.000 0.000 23.116
Approx polarizability: 55.309 13.410 91.121 0.000 0.000 30.957
Full mass-weighted force constant matrix:
Low frequencies --- -13.1930 -2.8046 -1.2104 -0.0004 0.0010 0.0012
Low frequencies --- 2.5468 4.6706 20.8447
****** 1 imaginary frequencies (negative Signs) ******
Harmonic frequencies (cm**-1), IR intensities (KM/Mole),
Raman scattering activities (A**4/AMU), Raman depolarization ratios,
reduced masses (AMU), force constants (mDyne/A) and normal coordinates:

	1	2	3
	?A	?A	A'
Frequencies --	-3.8849	1.5640	20.8279
Red. masses --	2.5606	6.4821	3.2824
Frc consts --	0.0000	0.0000	0.0008
IR Inten --	0.0157	0.4027	7.0216
Raman Activ --	0.0000	0.0000	0.0000
Depolar --	0.0000	0.0000	0.0000

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.00	0.00	0.03	0.07	0.01	0.00	-0.03	0.01	0.00
2	1	0.00	0.00	0.37	-0.07	-0.14	0.01	-0.08	-0.04	0.00
3	1	0.00	0.00	-0.45	0.00	0.20	-0.01	-0.05	0.08	0.00
4	6	0.00	0.00	-0.19	-0.28	0.08	0.00	0.03	-0.02	0.00
5	1	0.00	0.00	0.12	-0.21	0.13	0.00	0.18	0.09	0.00
6	1	0.00	0.00	-0.50	-0.26	-0.01	-0.01	0.07	-0.19	0.00
7	6	0.00	0.00	0.17	0.26	-0.13	0.00	-0.19	0.09	0.00

8	1	0.00	0.00	0.52	0.44	-0.01	0.01	-0.58	-0.18	0.00
9	1	0.00	0.00	-0.04	0.29	-0.35	0.00	-0.26	0.55	0.00
10	8	0.00	0.00	0.16	0.29	-0.04	0.00	0.05	0.00	0.00
11	8	0.00	0.00	-0.18	-0.37	0.11	0.00	-0.15	0.05	0.00
12	8	0.00	0.00	0.02	0.04	-0.03	0.00	0.28	-0.12	0.00

	4	5	6
	A"	A"	A"
Frequencies --	28.4197	50.1962	56.4313
Red. masses --	4.0143	3.2348	1.0662
Frc consts --	0.0019	0.0048	0.0020
IR Inten --	5.4865	0.0077	0.7139
Raman Activ --	0.0000	0.0000	0.0000
Depolar --	0.0000	0.0000	0.0000

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.00	0.00	0.15	0.00	0.00	0.26	0.00	0.00	0.05
2	1	0.00	0.00	0.24	0.00	0.00	0.28	0.00	0.00	0.58
3	1	0.00	0.00	0.35	0.00	0.00	0.64	0.00	0.00	-0.41
4	6	0.00	0.00	-0.16	0.00	0.00	-0.16	0.00	0.00	0.00
5	1	0.00	0.00	-0.32	0.00	0.00	-0.22	0.00	0.00	-0.02
6	1	0.00	0.00	-0.36	0.00	0.00	-0.20	0.00	0.00	0.05
7	6	0.00	0.00	0.20	0.00	0.00	-0.10	0.00	0.00	-0.02
8	1	0.00	0.00	0.38	0.00	0.00	-0.01	0.00	0.00	-0.53
9	1	0.00	0.00	0.47	0.00	0.00	-0.49	0.00	0.00	0.46
10	8	0.00	0.00	-0.15	0.00	0.00	-0.15	0.00	0.00	-0.04
11	8	0.00	0.00	0.22	0.00	0.00	-0.06	0.00	0.00	-0.02
12	8	0.00	0.00	-0.26	0.00	0.00	0.21	0.00	0.00	0.02

	7	8	9
	A'	A'	A"
Frequencies --	62.7567	72.1751	73.5062
Red. masses --	7.2512	2.5896	3.4528
Frc consts --	0.0168	0.0079	0.0110
IR Inten --	0.6825	0.8659	41.1903
Raman Activ --	0.0000	0.0000	0.0000
Depolar --	0.0000	0.0000	0.0000

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.13	0.32	0.00	0.19	-0.06	0.00	0.00	0.00	0.17
2	1	0.20	0.38	0.00	0.40	0.15	0.00	0.00	0.00	0.29
3	1	0.17	0.23	0.00	0.30	-0.34	0.00	0.00	0.00	0.31
4	6	0.01	0.01	0.00	-0.23	0.08	0.00	0.00	0.00	0.25
5	1	-0.03	-0.02	0.00	-0.47	-0.09	0.00	0.00	0.00	0.46
6	1	-0.01	0.05	0.00	-0.30	0.37	0.00	0.00	0.00	0.51
7	6	-0.13	-0.32	0.00	0.00	0.03	0.00	0.00	0.00	0.07
8	1	-0.15	-0.34	0.00	-0.09	-0.03	0.00	0.00	0.00	0.39
9	1	-0.13	-0.30	0.00	-0.02	0.14	0.00	0.00	0.00	-0.04
10	8	0.03	0.34	0.00	-0.12	0.00	0.00	0.00	0.00	-0.10
11	8	0.05	0.00	0.00	0.06	-0.03	0.00	0.00	0.00	-0.24
12	8	-0.10	-0.34	0.00	0.11	-0.02	0.00	0.00	0.00	-0.16

	10	11	12
	A'	A"	A'
Frequencies --	87.9401	102.6330	110.6397
Red. masses --	2.6908	1.0158	7.4399
Frc consts --	0.0123	0.0063	0.0537
IR Inten --	26.4933	0.2053	0.1787
Raman Activ --	0.0000	0.0000	0.0000
Depolar --	0.0000	0.0000	0.0000

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.21	-0.05	0.00	0.00	0.00	-0.01	-0.03	-0.21	0.00
2	1	0.45	0.19	0.00	0.00	0.00	0.25	-0.01	-0.19	0.00
3	1	0.34	-0.36	0.00	0.00	0.00	-0.28	-0.01	-0.24	0.00
4	6	0.14	-0.07	0.00	0.00	0.00	-0.01	0.13	0.38	0.00
5	1	0.40	0.12	0.00	0.00	0.00	-0.61	0.18	0.41	0.00
6	1	0.21	-0.39	0.00	0.00	0.00	0.56	0.14	0.34	0.00
7	6	0.01	0.01	0.00	0.00	0.00	0.00	-0.07	-0.18	0.00
8	1	0.08	0.05	0.00	0.00	0.00	0.29	-0.07	-0.18	0.00
9	1	0.02	-0.06	0.00	0.00	0.00	-0.29	-0.07	-0.18	0.00
10	8	-0.13	0.03	0.00	0.00	0.00	0.00	-0.06	-0.21	0.00
11	8	-0.19	0.05	0.00	0.00	0.00	0.02	0.09	0.40	0.00
12	8	-0.06	0.04	0.00	0.00	0.00	0.00	-0.07	-0.18	0.00

	13	14	15
	A"	A"	A"
Frequencies --	1207.0974	1220.0194	1222.4142
Red. masses --	1.3675	1.3620	1.3596
Frc consts --	1.1740	1.1944	1.1970
IR Inten --	2.8228	1.7807	2.9035

Raman Activ --		0.0000			0.0000			0.0000		
Depolar --		0.0000			0.0000			0.0000		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.00	0.00	0.00	0.00	0.00	-0.17	0.00	0.00	-0.02
2	1	0.00	0.00	0.00	0.00	0.00	0.69	0.00	0.00	0.07
3	1	0.00	0.00	0.00	0.00	0.00	0.69	0.00	0.00	0.06
4	6	0.00	0.00	0.00	0.00	0.00	0.02	0.00	0.00	-0.17
5	1	0.00	0.00	0.01	0.00	0.00	-0.06	0.00	0.00	0.69
6	1	0.00	0.00	0.01	0.00	0.00	-0.06	0.00	0.00	0.69
7	6	0.00	0.00	0.17	0.00	0.00	0.00	0.00	0.00	0.00
8	1	0.00	0.00	-0.70	0.00	0.00	0.00	0.00	0.00	0.01
9	1	0.00	0.00	-0.70	0.00	0.00	0.00	0.00	0.00	0.01
10	8	0.00	0.00	0.00	0.00	0.00	0.04	0.00	0.00	0.00
11	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.04
12	8	0.00	0.00	-0.04	0.00	0.00	0.00	0.00	0.00	0.00
		16			17			18		
		A'			A'			A'		
Frequencies --		1247.5158			1253.8389			1270.4956		
Red. masses --		1.3603			1.3566			1.3414		
Frc consts --		1.2473			1.2565			1.2757		
IR Inten --		30.9387			0.5857			9.8493		
Raman Activ --		0.0000			0.0000			0.0000		
Depolar --		0.0000			0.0000			0.0000		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.11	-0.02	0.00	-0.10	0.02	0.00	0.00	0.00	0.00
2	1	-0.28	-0.43	0.00	0.26	0.39	0.00	-0.01	-0.02	0.00
3	1	-0.09	0.51	0.00	0.08	-0.46	0.00	0.00	0.02	0.00
4	6	0.09	-0.03	0.00	0.10	-0.04	0.00	-0.02	0.01	0.00
5	1	-0.31	-0.34	0.00	-0.34	-0.38	0.00	0.08	0.09	0.00
6	1	-0.01	0.46	0.00	-0.01	0.51	0.00	0.00	-0.12	0.00
7	6	0.01	-0.01	0.00	0.02	-0.01	0.00	0.13	-0.06	0.00
8	1	-0.05	-0.05	0.00	-0.07	-0.07	0.00	-0.48	-0.49	0.00
9	1	0.00	0.07	0.00	0.00	0.10	0.00	0.03	0.69	0.00
10	8	-0.06	0.01	0.00	0.05	-0.01	0.00	0.00	0.00	0.00
11	8	-0.05	0.02	0.00	-0.05	0.02	0.00	0.01	0.00	0.00
12	8	-0.01	0.00	0.00	-0.01	0.00	0.00	-0.07	0.03	0.00
		19			20			21		
		A'			A'			A'		
Frequencies --		1525.2922			1528.8731			1539.7088		
Red. masses --		1.1098			1.1162			1.1099		
Frc consts --		1.5213			1.5372			1.5502		
IR Inten --		0.9135			67.2045			19.1092		
Raman Activ --		0.0000			0.0000			0.0000		
Depolar --		0.0000			0.0000			0.0000		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.00	0.01	0.00	0.00	0.01	0.00	0.00	0.00	0.00
2	1	0.34	0.38	0.00	0.32	0.36	0.00	0.01	0.02	0.00
3	1	-0.16	0.49	0.00	-0.15	0.46	0.00	-0.01	0.02	0.00
4	6	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00
5	1	-0.36	-0.31	0.00	0.39	0.32	0.00	0.10	0.09	0.00
6	1	0.08	-0.47	0.00	-0.09	0.49	0.00	-0.02	0.13	0.00
7	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00
8	1	0.06	0.05	0.00	-0.09	-0.07	0.00	0.56	0.41	0.00
9	1	-0.01	0.08	0.00	0.01	-0.11	0.00	-0.07	0.69	0.00
10	8	-0.01	-0.06	0.00	-0.01	-0.06	0.00	0.00	0.00	0.00
11	8	0.02	0.05	0.00	-0.02	-0.06	0.00	-0.01	-0.01	0.00
12	8	0.00	-0.01	0.00	0.00	0.01	0.00	-0.03	-0.07	0.00
		22			23			24		
		A'			A'			A'		
Frequencies --		1816.4858			1821.4805			1822.8393		
Red. masses --		6.9537			7.1708			7.3714		
Frc consts --		13.5185			14.0174			14.4311		
IR Inten --		342.1256			23.9412			58.8671		
Raman Activ --		0.0000			0.0000			0.0000		
Depolar --		0.0000			0.0000			0.0000		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.04	0.20	0.00	0.11	0.53	0.00	0.00	0.00	0.00
2	1	-0.19	-0.07	0.00	-0.45	-0.12	0.00	0.00	0.00	0.00
3	1	0.14	-0.14	0.00	0.37	-0.29	0.00	0.00	0.00	0.00
4	6	0.17	0.48	0.00	-0.07	-0.18	0.00	-0.06	-0.17	0.00
5	1	-0.44	-0.06	0.00	0.17	0.02	0.00	0.14	0.00	0.00
6	1	0.30	-0.33	0.00	-0.12	0.13	0.00	-0.11	0.09	0.00
7	6	0.07	0.15	0.00	-0.03	-0.06	0.00	0.23	0.51	0.00
8	1	-0.14	-0.01	0.00	0.06	0.00	0.00	-0.47	-0.02	0.00

9	1	0.09	-0.11	0.00	-0.04	0.04	0.00	0.30	-0.36	0.00	
10	8	-0.03	-0.14	0.00	-0.08	-0.37	0.00	0.00	0.00	0.00	
11	8	-0.12	-0.33	0.00	0.05	0.13	0.00	0.05	0.12	0.00	
12	8	-0.05	-0.11	0.00	0.02	0.04	0.00	-0.16	-0.36	0.00	

	25	26	27
	A'	A'	A'
Frequencies --	2887.7799	2895.5426	2909.3643
Red. masses --	1.0438	1.0440	1.0447
Frc consts --	5.1284	5.1570	5.2100
IR Inten --	89.2191	67.7082	52.4160
Raman Activ --	0.0000	0.0000	0.0000
Depolar --	0.0000	0.0000	0.0000

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.00	0.00	0.00	-0.01	-0.06	0.00	0.00	0.01	0.00
2	1	-0.02	0.02	0.00	-0.52	0.47	0.00	0.05	-0.04	0.00
3	1	0.03	0.01	0.00	0.67	0.23	0.00	-0.06	-0.02	0.00
4	6	0.00	0.00	0.00	0.00	0.00	0.00	-0.02	-0.05	0.00
5	1	-0.03	0.03	0.00	-0.04	0.05	0.00	-0.44	0.53	0.00
6	1	0.04	0.01	0.00	0.06	0.01	0.00	0.70	0.13	0.00
7	6	-0.02	-0.05	0.00	0.00	0.00	0.00	0.00	0.00	0.00
8	1	-0.41	0.56	0.00	0.02	-0.03	0.00	0.02	-0.03	0.00
9	1	0.70	0.08	0.00	-0.04	0.00	0.00	-0.04	0.00	0.00
10	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
11	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
12	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

	28	29	30
	A'	A'	A'
Frequencies --	2947.2173	2954.4525	2975.4354
Red. masses --	1.1212	1.1203	1.1208
Frc consts --	5.7377	5.7613	5.8465
IR Inten --	117.9459	126.3447	129.4722
Raman Activ --	0.0000	0.0000	0.0000
Depolar --	0.0000	0.0000	0.0000

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.00	0.00	0.00	-0.10	0.02	0.00	0.00	0.00	0.00
2	1	-0.01	0.01	0.00	0.51	-0.50	0.00	0.02	-0.02	0.00
3	1	-0.01	0.00	0.00	0.65	0.25	0.00	0.03	0.01	0.00
4	6	0.00	0.00	0.00	0.00	0.00	0.00	-0.09	0.04	0.00
5	1	-0.02	0.02	0.00	-0.02	0.03	0.00	0.44	-0.57	0.00
6	1	-0.02	-0.01	0.00	-0.03	-0.01	0.00	0.67	0.15	0.00
7	6	-0.09	0.04	0.00	0.00	0.00	0.00	0.00	0.00	0.00
8	1	0.40	-0.58	0.00	0.01	-0.01	0.00	0.01	-0.02	0.00
9	1	0.69	0.10	0.00	0.01	0.00	0.00	0.02	0.00	0.00
10	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
11	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
12	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

- Thermochemistry -

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Atom 1 has atomic number 6 and mass 12.00000
Atom 2 has atomic number 1 and mass 1.00783
Atom 3 has atomic number 1 and mass 1.00783
Atom 4 has atomic number 6 and mass 12.00000
Atom 5 has atomic number 1 and mass 1.00783
Atom 6 has atomic number 1 and mass 1.00783
Atom 7 has atomic number 6 and mass 12.00000
Atom 8 has atomic number 1 and mass 1.00783
Atom 9 has atomic number 1 and mass 1.00783
Atom 10 has atomic number 8 and mass 15.99491
Atom 11 has atomic number 8 and mass 15.99491
Atom 12 has atomic number 8 and mass 15.99491
Molecular mass: 90.03169 amu.
Principal axes and moments of inertia in atomic units:

	1	2	3
EIGENVALUES --	25.735734	091.993434	117.72916
X	0.28501	0.95852	0.00000
Y	0.95852	-0.28501	0.00000
Z	0.00000	0.00000	1.00000

THIS MOLECULE IS AN ASYMMETRIC TOP.
ROTATIONAL SYMMETRY NUMBER 1.
ROTATIONAL TEMPERATURES (KELVIN) 3.36549 0.02117 0.02103
ROTATIONAL CONSTANTS (GHZ) 70.12591 0.44104 0.43829

1 IMAGINARY FREQUENCIES IGNORED.
Zero-point vibrational energy 213610.9 (Joules/Mol)
51.05422 (Kcal/Mol)
WARNING-- EXPLICIT CONSIDERATION OF 11 DEGREES OF FREEDOM AS
VIBRATIONS MAY CAUSE SIGNIFICANT ERROR
VIBRATIONAL TEMPERATURES: 2.25 29.97 40.89 72.22 81.19
(KELVIN) 90.29 103.84 105.76 126.53 147.67
159.18 1736.73 1755.33 1758.77 1794.89
1803.98 1827.95 2194.54 2199.69 2215.28
2613.50 2620.69 2622.64 4154.85 4166.02
4185.90 4240.36 4250.77 4280.96

Zero-point correction= 0.081360 (Hartree/Particle)
Thermal correction to Energy= 0.093258
Thermal correction to Enthalpy= 0.094202
Thermal correction to Gibbs Free Energy= 0.035435
Sum of electronic and zero-point Energies= -343.536340
Sum of electronic and thermal Energies= -343.524442
Sum of electronic and thermal Enthalpies= -343.523498
Sum of electronic and thermal Free Energies= -343.582265

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	58.520	28.990	123.685
ELECTRONIC	0.000	0.000	0.000
TRANSLATIONAL	0.889	2.981	39.405
ROTATIONAL	0.889	2.981	27.564
VIBRATIONAL	56.743	23.029	56.716
VIBRATION 1	0.592	1.987	11.698
VIBRATION 2	0.593	1.986	6.554
VIBRATION 3	0.593	1.984	5.937
VIBRATION 4	0.595	1.978	4.810
VIBRATION 5	0.596	1.975	4.578
VIBRATION 6	0.597	1.972	4.369
VIBRATION 7	0.598	1.967	4.093
VIBRATION 8	0.599	1.967	4.057
VIBRATION 9	0.601	1.958	3.705
VIBRATION 10	0.605	1.947	3.404
VIBRATION 11	0.606	1.941	3.258

	Q	LOG10(Q)	LN(Q)
TOTAL BOT	0.502324D-16	-16.299016	-37.529872
TOTAL V=0	0.132975D+22	21.123769	48.639276
VIB (BOT)	0.634623D-29	-29.197484	-67.229691
VIB (BOT) 1	0.132498D+03	2.122210	4.886570
VIB (BOT) 2	0.994526D+01	0.997616	2.297096
VIB (BOT) 3	0.728591D+01	0.862484	1.985942
VIB (BOT) 4	0.411824D+01	0.614712	1.415427
VIB (BOT) 5	0.366086D+01	0.563583	1.297697
VIB (BOT) 6	0.328947D+01	0.517125	1.190725
VIB (BOT) 7	0.285669D+01	0.455864	1.049665
VIB (BOT) 8	0.280443D+01	0.447845	1.031202
VIB (BOT) 9	0.233885D+01	0.369003	0.849661
VIB (BOT) 10	0.199861D+01	0.300727	0.692450
VIB (BOT) 11	0.185092D+01	0.267387	0.615681
VIB (V=0)	0.167997D+09	8.225301	18.939457
VIB (V=0) 1	0.132999D+03	2.123849	4.890344
VIB (V=0) 2	0.104578D+02	1.019441	2.347350
VIB (V=0) 3	0.780304D+01	0.892264	2.054514
VIB (V=0) 4	0.464848D+01	0.667311	1.536541
VIB (V=0) 5	0.419484D+01	0.622716	1.433856
VIB (V=0) 6	0.382725D+01	0.582887	1.342146
VIB (V=0) 7	0.340012D+01	0.531494	1.223811
VIB (V=0) 8	0.334866D+01	0.524871	1.208560
VIB (V=0) 9	0.289170D+01	0.461153	1.061845
VIB (V=0) 10	0.256020D+01	0.408274	0.940085
VIB (V=0) 11	0.241726D+01	0.383324	0.882635
ELECTRONIC	0.100000D+01	0.000000	0.000000
TRANSLATIONAL	0.335779D+08	7.526054	17.329379
ROTATIONAL	0.235729D+06	5.372414	12.370440

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

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z

1	6	0.000007494	-0.000017703	0.000000000
2	1	0.000045349	0.000032966	0.000000000
3	1	0.000000485	-0.000000226	0.000000000
4	6	0.000038209	-0.000059614	0.000000000
5	1	0.000006956	-0.000005715	0.000000000
6	1	0.000001131	-0.000040573	0.000000000
7	6	-0.000004044	-0.000068195	0.000000000
8	1	-0.000007183	0.000008657	0.000000000
9	1	0.000011429	-0.000002815	0.000000000
10	8	-0.000001352	0.000022776	0.000000000
11	8	-0.000098748	-0.000009292	0.000000000
12	8	0.000000274	0.000139734	0.000000000

Cartesian Forces: Max 0.000139734 RMS 0.000035383

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Internal Forces: Max 0.000052541 RMS 0.000016568
Search for a local minimum.
Step number 1 out of a maximum of 63
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Second derivative matrix not updated -- analytic derivatives used.
Eigenvalues --- 0.00000 0.00000 0.00002 0.00004 0.00005
Eigenvalues --- 0.00008 0.00018 0.00022 0.00069 0.00086
Eigenvalues --- 0.00155 0.00169 0.02494 0.03949 0.04748
Eigenvalues --- 0.08046 0.08096 0.12413 0.13046 0.13117
Eigenvalues --- 0.18839 0.27536 0.27834 0.29163 0.29576
Eigenvalues --- 0.29786 0.30525 0.88007 0.88514 0.89146
Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
Eigenvalues --- 1000.000001000.000001000.00000
Eigenvalue 1 out of range, new value = 0.000000 Eigenvector:

	1
R1	0.00000
R2	0.00000
R3	0.00000
R4	0.00000
R5	0.00000
R6	0.00000
R7	0.00000
R8	0.00000
R9	0.00000
R10	0.00000
R11	0.00000
R12	0.00000
R13	0.00000
R14	0.00000
R15	0.00000
A1	0.00000
A2	0.00000
A3	0.00000
A4	0.00000
A5	0.00000
A6	0.00000
A7	0.00000
A8	0.00000
A9	0.00000
A10	0.00000
A11	-0.00001
A12	0.00000
A13	0.00001
A14	-0.00001
A15	0.00000
A16	0.00000
A17	0.00000
A18	0.00000
A19	0.00000
A20	-0.00280
A21	-0.00223
D1	0.99832
D2	-0.02126
D3	0.01269

D4	-0.00289
D5	-0.02124
D6	0.01271
D7	-0.00287
D8	-0.02651
D9	0.01783
D10	-0.00500
D11	-0.02510
D12	0.01924
D13	-0.00360
D14	0.00370
D15	-0.00186
D16	0.00370
D17	-0.00186

Quadratic step=6.212D-01 exceeds max=3.000D-01 adjusted using Lamda=-5.339D-05.
Angle between NR and scaled steps= 11.88 degrees.
Angle between quadratic step and forces= 59.55 degrees.
Linear search not attempted -- first point.
Iteration 1 RMS(Cart)= 0.01474672 RMS(Int)= 0.03710659
Iteration 2 RMS(Cart)= 0.00048796 RMS(Int)= 0.03697001
Iteration 3 RMS(Cart)= 0.00048262 RMS(Int)= 0.03683492
Iteration 4 RMS(Cart)= 0.00047738 RMS(Int)= 0.03670129
Iteration 5 RMS(Cart)= 0.00047224 RMS(Int)= 0.03656909
Iteration 6 RMS(Cart)= 0.00046718 RMS(Int)= 0.03643831
Iteration 7 RMS(Cart)= 0.00046222 RMS(Int)= 0.03630891
Iteration 8 RMS(Cart)= 0.00045734 RMS(Int)= 0.03618087
Iteration 9 RMS(Cart)= 0.00045255 RMS(Int)= 0.03605417
Iteration 10 RMS(Cart)= 0.00044784 RMS(Int)= 0.03592879
Iteration 11 RMS(Cart)= 0.00044322 RMS(Int)= 0.03580469
Iteration 12 RMS(Cart)= 0.00043867 RMS(Int)= 0.03568187
Iteration 13 RMS(Cart)= 0.00043420 RMS(Int)= 0.03556029
Iteration 14 RMS(Cart)= 0.00042980 RMS(Int)= 0.03543994
Iteration 15 RMS(Cart)= 0.00042548 RMS(Int)= 0.03532080
Iteration 16 RMS(Cart)= 0.00042123 RMS(Int)= 0.03520284
Iteration 17 RMS(Cart)= 0.00041704 RMS(Int)= 0.03508606
Iteration 18 RMS(Cart)= 0.00041293 RMS(Int)= 0.03497042
Iteration 19 RMS(Cart)= 0.00040889 RMS(Int)= 0.03485591
Iteration 20 RMS(Cart)= 0.00040491 RMS(Int)= 0.03474251
Iteration 21 RMS(Cart)= 0.00040099 RMS(Int)= 0.03463020
Iteration 22 RMS(Cart)= 0.00039714 RMS(Int)= 0.03451897
Iteration 23 RMS(Cart)= 0.00039335 RMS(Int)= 0.03440880
Iteration 24 RMS(Cart)= 0.00038962 RMS(Int)= 0.03429967
Iteration 25 RMS(Cart)= 0.00038594 RMS(Int)= 0.03419157
Iteration 26 RMS(Cart)= 0.00038233 RMS(Int)= 0.03408448
Iteration 27 RMS(Cart)= 0.00037877 RMS(Int)= 0.03397838
Iteration 28 RMS(Cart)= 0.00037526 RMS(Int)= 0.03387326
Iteration 29 RMS(Cart)= 0.00037181 RMS(Int)= 0.03376911
Iteration 30 RMS(Cart)= 0.00036841 RMS(Int)= 0.03366590
Iteration 31 RMS(Cart)= 0.00036507 RMS(Int)= 0.03356363
Iteration 32 RMS(Cart)= 0.00036177 RMS(Int)= 0.03346229
Iteration 33 RMS(Cart)= 0.00035852 RMS(Int)= 0.03336184
Iteration 34 RMS(Cart)= 0.00035532 RMS(Int)= 0.03326230
Iteration 35 RMS(Cart)= 0.00035217 RMS(Int)= 0.03316363
Iteration 36 RMS(Cart)= 0.00034906 RMS(Int)= 0.03306583
Iteration 37 RMS(Cart)= 0.00034600 RMS(Int)= 0.03296889
Iteration 38 RMS(Cart)= 0.00034299 RMS(Int)= 0.03287279
Iteration 39 RMS(Cart)= 0.00034001 RMS(Int)= 0.03277752
Iteration 40 RMS(Cart)= 0.00033708 RMS(Int)= 0.03268307
Iteration 41 RMS(Cart)= 0.00033419 RMS(Int)= 0.03258943
Iteration 42 RMS(Cart)= 0.00033135 RMS(Int)= 0.03249658
Iteration 43 RMS(Cart)= 0.00032854 RMS(Int)= 0.03240452
Iteration 44 RMS(Cart)= 0.00032577 RMS(Int)= 0.03231323
Iteration 45 RMS(Cart)= 0.00032304 RMS(Int)= 0.03222271
Iteration 46 RMS(Cart)= 0.00032035 RMS(Int)= 0.03213294
Iteration 47 RMS(Cart)= 0.00031770 RMS(Int)= 0.03204391
Iteration 48 RMS(Cart)= 0.00031508 RMS(Int)= 0.03195561
Iteration 49 RMS(Cart)= 0.00031250 RMS(Int)= 0.03186803
Iteration 50 RMS(Cart)= 0.00030995 RMS(Int)= 0.03178117
Iteration 51 RMS(Cart)= 0.00030744 RMS(Int)= 0.03169500
Iteration 52 RMS(Cart)= 0.00030496 RMS(Int)= 0.03160953
Iteration 53 RMS(Cart)= 0.00030251 RMS(Int)= 0.03152475
Iteration 54 RMS(Cart)= 0.00030010 RMS(Int)= 0.03144064
Iteration 55 RMS(Cart)= 0.00029772 RMS(Int)= 0.03135719
Iteration 56 RMS(Cart)= 0.00029537 RMS(Int)= 0.03127441

Iteration 57 RMS(Cart)= 0.00029305 RMS(Int)= 0.03119227
Iteration 58 RMS(Cart)= 0.00029076 RMS(Int)= 0.03111077
Iteration 59 RMS(Cart)= 0.00028850 RMS(Int)= 0.03102990
Iteration 60 RMS(Cart)= 0.00028627 RMS(Int)= 0.03094966
Iteration 61 RMS(Cart)= 0.00028407 RMS(Int)= 0.03087003
Iteration 62 RMS(Cart)= 0.00028189 RMS(Int)= 0.03079102
Iteration 63 RMS(Cart)= 0.00027975 RMS(Int)= 0.03071260
Iteration 64 RMS(Cart)= 0.00027763 RMS(Int)= 0.03063477
Iteration 65 RMS(Cart)= 0.00027554 RMS(Int)= 0.03055753
Iteration 66 RMS(Cart)= 0.00027347 RMS(Int)= 0.03048087
Iteration 67 RMS(Cart)= 0.00027143 RMS(Int)= 0.03040478
Iteration 68 RMS(Cart)= 0.00026941 RMS(Int)= 0.03032925
Iteration 69 RMS(Cart)= 0.00026742 RMS(Int)= 0.03025428
Iteration 70 RMS(Cart)= 0.00026546 RMS(Int)= 0.03017986
Iteration 71 RMS(Cart)= 0.00026351 RMS(Int)= 0.03010599
Iteration 72 RMS(Cart)= 0.00026159 RMS(Int)= 0.03003265
Iteration 73 RMS(Cart)= 0.00025970 RMS(Int)= 0.02995984
Iteration 74 RMS(Cart)= 0.00025783 RMS(Int)= 0.02988755
Iteration 75 RMS(Cart)= 0.00025597 RMS(Int)= 0.02981579
Iteration 76 RMS(Cart)= 0.00025415 RMS(Int)= 0.02974453
Iteration 77 RMS(Cart)= 0.00025234 RMS(Int)= 0.02967378
Iteration 78 RMS(Cart)= 0.00025055 RMS(Int)= 0.02960353
Iteration 79 RMS(Cart)= 0.00024879 RMS(Int)= 0.02953378
Iteration 80 RMS(Cart)= 0.00024704 RMS(Int)= 0.02946451
Iteration 81 RMS(Cart)= 0.00024532 RMS(Int)= 0.02939572
Iteration 82 RMS(Cart)= 0.00024362 RMS(Int)= 0.02932741
Iteration 83 RMS(Cart)= 0.00024193 RMS(Int)= 0.02925958
Iteration 84 RMS(Cart)= 0.00024027 RMS(Int)= 0.02919220
Iteration 85 RMS(Cart)= 0.00023862 RMS(Int)= 0.02912529
Iteration 86 RMS(Cart)= 0.00023699 RMS(Int)= 0.02905884
Iteration 87 RMS(Cart)= 0.00023538 RMS(Int)= 0.02899283
Iteration 88 RMS(Cart)= 0.00023379 RMS(Int)= 0.02892727
Iteration 89 RMS(Cart)= 0.00023222 RMS(Int)= 0.02886215
Iteration 90 RMS(Cart)= 0.00023067 RMS(Int)= 0.02879747
Iteration 91 RMS(Cart)= 0.00022913 RMS(Int)= 0.02873322
Iteration 92 RMS(Cart)= 0.00022761 RMS(Int)= 0.02866939
Iteration 93 RMS(Cart)= 0.00022610 RMS(Int)= 0.02860598
Iteration 94 RMS(Cart)= 0.00022461 RMS(Int)= 0.02854299
Iteration 95 RMS(Cart)= 0.00022314 RMS(Int)= 0.02848042
Iteration 96 RMS(Cart)= 0.00022169 RMS(Int)= 0.02841824
Iteration 97 RMS(Cart)= 0.00022025 RMS(Int)= 0.02835648
Iteration 98 RMS(Cart)= 0.00021882 RMS(Int)= 0.02829511
Iteration 99 RMS(Cart)= 0.00021741 RMS(Int)= 0.02823414
Iteration100 RMS(Cart)= 0.00021602 RMS(Int)= 0.02817355
Curvilinear step not converged.

Variable	Old X	-DE/DX (Linear)	Delta X (Quad)	Delta X (Total)	Delta X	New X
R1	2.09312	0.00001	0.00000	-0.00012	0.00007	2.09318
R2	2.09320	0.00000	0.00000	0.00013	0.00015	2.09335
R3	2.27217	0.00002	0.00000	0.00011	0.00015	2.27232
R4	5.86058	0.00001	0.00000	-0.00431	-0.00110	5.85948
R5	5.03565	0.00005	0.00000	-0.01464	-0.00441	5.03124
R6	5.05518	-0.00001	0.00000	0.00715	0.00249	5.05768
R7	2.09048	0.00000	0.00000	-0.00001	0.00001	2.09049
R8	2.09075	0.00000	0.00000	-0.00006	-0.00001	2.09074
R9	2.27443	0.00000	0.00000	-0.00001	0.00001	2.27445
R10	5.87635	-0.00003	0.00000	-0.01915	-0.00603	5.87032
R11	5.05349	0.00001	0.00000	-0.01307	-0.00411	5.04938
R12	5.08390	-0.00005	0.00000	-0.02326	-0.00733	5.07656
R13	2.09397	-0.00001	0.00000	-0.00001	0.00013	2.09410
R14	2.09400	-0.00001	0.00000	-0.00010	0.00010	2.09411
R15	2.27111	0.00005	0.00000	0.00008	0.00017	2.27129
A1	1.99849	0.00001	0.00000	0.00028	0.00009	1.99858
A2	2.14241	0.00000	0.00000	0.00012	0.00004	2.14245
A3	2.14229	-0.00001	0.00000	-0.00040	-0.00013	2.14216
A4	3.13687	0.00002	0.00000	-0.00508	-0.00161	3.13527
A5	2.00626	0.00000	0.00000	-0.00020	-0.00007	2.00620
A6	2.13799	0.00001	0.00000	0.00067	0.00021	2.13820
A7	2.13893	-0.00001	0.00000	-0.00046	-0.00015	2.13878
A8	2.02228	0.00000	0.00000	0.00006	0.00002	2.02230
A9	2.13016	0.00000	0.00000	0.00037	0.00012	2.13027
A10	2.13075	0.00000	0.00000	-0.00043	-0.00014	2.13061
A11	2.99060	0.00002	0.00000	0.14696	0.04654	3.03714
A12	0.71284	0.00000	0.00000	0.00060	0.00019	0.71303

A13	2.93660	-0.00003	0.00000	-0.14676	-0.04648	2.89012
A14	2.63375	0.00002	0.00000	0.14616	0.04628	2.68003
A15	0.71035	0.00000	0.00000	0.00261	0.00083	0.71118
A16	2.85931	-0.00003	0.00000	-0.09115	-0.02886	2.83045
A17	2.71352	0.00002	0.00000	0.08853	0.02803	2.74156
A18	3.14951	-0.00003	0.00000	-0.00306	-0.00097	3.14855
A19	3.06937	0.00002	0.00000	0.08962	0.02838	3.09775
A20	3.14159	0.00000	0.00000	0.00005	0.00000	3.14159
A21	3.14159	0.00000	0.00000	0.00003	0.00000	3.14159
D1	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D2	3.14159	0.00000	0.00000	-0.00005	0.00000	3.14159
D3	0.00000	0.00000	0.00000	0.00001	0.00000	0.00000
D4	3.14159	0.00000	0.00000	-0.00002	0.00000	3.14159
D5	0.00000	0.00000	0.00000	-0.00005	0.00000	0.00000
D6	3.14159	0.00000	0.00000	0.00001	0.00000	3.14159
D7	0.00000	0.00000	0.00000	-0.00002	0.00000	0.00000
D8	3.14159	0.00000	0.00000	0.00010	0.00000	3.14159
D9	0.00000	0.00000	0.00000	-0.00002	0.00000	0.00000
D10	3.14159	0.00000	0.00000	0.00005	0.00000	3.14159
D11	0.00000	0.00000	0.00000	0.00008	0.00000	0.00000
D12	3.14159	0.00000	0.00000	-0.00004	0.00000	3.14159
D13	0.00000	0.00000	0.00000	0.00003	0.00000	0.00000
D14	0.00000	0.00000	0.00000	0.00001	0.00000	0.00000
D15	3.14159	0.00000	0.00000	0.00005	0.00000	3.14159
D16	3.14159	0.00000	0.00000	0.00001	0.00000	3.14159
D17	0.00000	0.00000	0.00000	0.00005	0.00000	0.00000

Item	Value	Threshold	Converged?
Maximum Force	0.000053	0.000450	YES
RMS Force	0.000017	0.000300	YES
Maximum Displacement	0.132996	0.001800	NO
RMS Displacement	0.046620	0.001200	NO

Predicted change in Energy=-7.116268D-07
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

1|1|UNPC-UNK|Freq|RB3LYP|CBSB7|C3H6O3|PCUSER|11-Oct-2015|0||#N GEOM=AL
LCHECK GUESS=TCHECK B3LYP/CBSB7 FREQ||Title Card Required||0,1|C,1.563
7698791,3.4284420444,0.|H,2.2282278702,2.5422482383,0.|H,0.481755476,3
.1913956349,0.|C,-0.0820898157,-0.5386793693,0.|H,0.4497309692,-1.5086
906652,0.|H,-1.1860533013,-0.6116939792,0.|C,-2.2018717885,-4.29043128
43,0.|H,-1.7248430438,-5.2905769429,0.|H,-3.3099473356,-4.2832988636,0
.|O,1.9826278561,4.5555092219,0.|O,0.4971437781,0.5163517725,0.|O,-1.5
569866697,-3.2762824654,0.||Version=x86-Win32-G98RevA.11.4|State=1-A'|
HF=-343.6177|RMSD=1.952e-009|RMSF=3.538e-005|Dipole=-1.4002577,-2.7648
656,0.|DipoleDeriv=0.8528787,0.1168472,0.0000086,0.1246549,1.1056207,0
.0000188,0.0000002,0.0000003,0.1648696,-0.0939426,0.1896956,0.000001,0
.1266231,-0.1095948,-0.0000051,-0.0000126,-0.0000123,0.071217,-0.26696
38,-0.0652297,-0.000008,0.0047972,0.0543874,-0.000005,0.000013,0.00001
23,0.0692312,0.8753875,0.2065833,-0.0000047,0.1942218,1.1361325,-0.000
0189,-0.0000065,-0.000007,0.176318,-0.0397361,0.1694326,0.0000021,0.09
6278,-0.1592262,0.0000018,0.0000191,0.0000175,0.0732875,-0.2448714,-0.
0377142,-0.0000045,0.0451047,0.0472986,0.0000029,-0.0000071,-0.0000052
,0.0722935,0.9317981,0.1508874,-0.0000218,0.1406967,1.0774839,-0.00001
45,0.000001,0.0000013,0.1800144,-0.0582048,0.1244404,0.0000074,0.08299
72,-0.2117002,-0.0000104,-0.0000047,-0.0000063,0.0777305,-0.2604314,-0
.01551,0.0000008,0.0316893,-0.0058557,0.0000013,0.0000044,0.0000053,0.
0778187,-0.5153994,-0.2008287,-0.0000016,-0.2100473,-0.9738803,-0.0000
093,-0.0000005,-0.0000002,-0.3320679,-0.5749974,-0.3250449,0.0000073,-
0.3269494,-1.036302,0.0000155,-0.000005,-0.0000048,-0.32096,-0.6055175
,-0.3135589,0.0000133,-0.3100661,-0.9243638,0.0000228,-0.0000012,-0.00
00009,-0.3097525|Polar=46.6289354,10.5673091,62.4840262,-0.0002791,-0.
0003039,23.1164505|PG=CS [SG(C3H6O3)]||NImag=1||0.63020900,0.13390753,0
.94183930,0.00000003,0.00000006,0.17788203,-0.16485221,0.10116149,0.,0
.15342753,0.11013502,-0.16750009,-0.00000002,-0.11581240,0.21480808,-0
.00000004,-0.00000011,-0.05997609,0.,0.00000004,0.02041973,-0.27018447
,-0.01197982,-0.00000003,-0.01691165,-0.00279546,0.00000004,0.29398597
,-0.02119569,-0.06168615,-0.00000001,0.02146145,0.00485503,0.00000007,
0.04737485,0.07386069,-0.00000007,-0.00000011,-0.05994706,-0.00000002,
0.00000002,0.02030416,0.00000005,-0.00000002,0.02040171,-0.00103152,-0
.00122698,-0.00000003,-0.00026243,0.00002503,-0.00000015,0.00052692,-0
.00084357,0.00000026,0.68043261,-0.00137447,-0.00311707,-0.00000006,-0
.00090846,-0.00040886,0.00000022,0.00054972,-0.00067422,-0.00000004,0.
17028429,0.89833845,-0.00000019,-0.00000041,0.00003692,-0.00000002,0.0
0000011,0.00002297,0.00000017,0.00000011,0.00004217,0.00000010,0.00000
042,0.17806789,-0.00000689,-0.00017528,0.,-0.00001263,-0.00003621,-0.0

0000004,-0.00002837,0.00011753,0.00000002,-0.13642045,0.09917842,-0.00
000005,0.12312839,0.00066831,0.00031296,0.,0.00014010,0.00011645,0.,-0
.00031847,0.00033329,-0.00000002,0.10720940,-0.20070085,-0.00000004,-0
.10407130,0.24878270,-0.00000023,-0.00000044,-0.00000014,-0.00000005,0
.00000010,-0.00002742,0.00000020,0.00000002,0.00010775,0.00000052,0.00
000018,-0.06012199,0.00000002,-0.00000006,0.02062263,-0.00014085,0.000
58346,0.,0.00030452,0.00000384,0.00000017,-0.00004799,0.00019304,-0.00
000017,-0.27497054,0.01859068,0.00000010,-0.01309147,-0.00049573,-0.00
000024,0.30631032,-0.00033175,0.00025942,0.,0.00029842,0.00008393,-0.0
0000007,0.00002467,0.00001839,0.00000006,0.01051023,-0.06153646,-0.000
00006,0.02399242,0.00198036,0.00000007,0.01294713,0.06491004,0.0000004
3,0.00000090,-0.00000485,0.00000007,-0.00000023,0.00008921,-0.00000039
,-0.00000016,-0.00004194,-0.00000055,-0.00000069,-0.06014569,0.0000000
5,0.00000010,0.02033567,0.00000006,0.00000003,0.02059682,-0.00003252,-
0.00036744,-0.00000005,-0.00011966,0.00000143,0.00000039,0.00004071,-0
.00007795,-0.00000023,-0.00121903,-0.00143154,0.00000049,-0.00025316,0
.00004056,-0.00000012,0.00031443,-0.00086951,-0.00000053,0.69680085,-0
.00033346,-0.00060962,-0.00000007,-0.00013795,-0.00000774,-0.00000026,
0.00016879,-0.00010353,0.00000054,-0.00144684,-0.00273486,0.00000030,-
0.00099090,-0.00026653,0.00000113,0.00033940,-0.00060471,-0.00000132,0
.18689524,0.87240105,0.00000008,0.00000016,0.00000569,0.00000001,-0.00
000004,0.00000395,-0.00000007,-0.00000004,0.00000395,-0.00000006,-0.00
000015,0.00003897,0.00000001,0.00000002,0.00003235,-0.00000002,0.00000
002,0.00003997,-0.00000016,-0.00000017,0.17565931,-0.00002710,-0.00002
372,0.00000001,0.00000257,0.00000379,-0.00000025,0.00001286,0.00000604
,0.00000023,0.00007331,-0.00009218,-0.00000017,-0.00001466,-0.00003042
,0.00000031,-0.00003126,0.00015236,-0.00000003,-0.12521620,0.09456329,
0.00000004,0.11188097,0.00009829,0.00014575,0.,0.00002683,-0.00000229,
0.00000046,-0.00005187,0.00001505,-0.00000047,0.00072005,0.00023932,0.
00000024,0.00018216,0.00009707,-0.00000069,-0.00026657,0.00038105,0.00
000025,0.09822241,-0.20735685,-0.00000004,-0.09386389,0.25611018,-0.00
000044,-0.00000094,0.00000192,-0.00000006,0.00000025,0.00000131,0.0000
0040,0.00000022,0.00000141,0.00000038,0.00000085,0.00000515,-0.0000000
8,-0.00000010,-0.00003198,0.00000010,-0.00000009,0.00009936,0.00000086
,0.00000101,-0.05894580,-0.00000019,0.00000018,0.01989587,0.00000437,0
.00010635,0.,0.00003622,-0.00000080,0.,-0.00001092,0.00002236,0.,-0.00
007891,0.00066573,-0.00000002,0.00033255,-0.00003020,0.,-0.00001330,0.
00019762,0.00000003,-0.26644244,0.03191592,0.,-0.01057706,0.00142693,-
0.00000004,0.30212363,0.00001209,0.00004267,0.,0.00001438,0.00000001,0
.00000002,-0.00001038,0.00000908,-0.00000005,-0.00023314,0.00033812,-0
.00000003,0.00031782,0.00004389,-0.00000010,0.00000026,0.00003191,0.00
000012,0.02819651,-0.06601948,0.00000002,0.02416229,0.00143894,-0.0000
0009,-0.00457099,0.06573458,0.00000026,0.00000057,0.00000181,0.0000000
3,-0.00000015,0.00000130,-0.00000024,-0.00000014,0.00000122,-0.0000002
0,-0.00000053,-0.00000293,0.00000005,0.00000006,0.00009469,-0.00000008
,0.00000007,-0.00003604,-0.00000056,-0.00000056,-0.05897883,0.00000015
,-0.00000017,0.01975974,0.00000002,0.00000005,0.01989308,-0.19223320,-
0.22348484,0.,0.02735495,0.00942683,-0.00000001,-0.00731325,-0.0476112
8,0.00000003,0.00063552,0.00109462,0.00000003,0.00002762,-0.00036156,0
.00000008,-0.00005989,0.00004570,-0.00000011,0.00008082,0.00023860,-0.
00000002,0.00001062,-0.00005804,0.00000009,-0.00002092,-0.00001178,-0.
00000005,0.17152214,-0.22335424,-0.71075757,-0.00000003,-0.00754264,-0
.05156008,0.00000002,-0.03093363,-0.01693823,0.00000010,0.00140915,0.0
0273552,0.00000020,0.00007758,-0.00050349,0.00000030,-0.00052143,-0.00
021294,-0.00000050,0.00033680,0.00056270,-0.00000009,0.00001511,-0.000
12601,0.00000049,-0.00009637,-0.00003832,-0.00000029,0.26269854,0.7808
4606,0.00000008,0.00000017,-0.05845036,0.00000001,-0.00000004,0.019562
10,-0.00000007,-0.00000003,0.01957505,-0.00000009,-0.00000014,-0.00004
285,0.00000001,0.00000002,-0.00000707,0.,0.,-0.00001259,-0.00000012,-0
.00000022,-0.00000870,0.,0.00000002,-0.00000301,0.,0.00000002,-0.00000
284,-0.00000002,-0.00000009,0.01934275,-0.00177593,0.00110827,0.000000
03,0.00090713,-0.00095327,0.00000003,-0.00000985,0.00047298,-0.0000001
3,-0.26637970,-0.28790147,-0.00000016,0.02553402,-0.00167699,-0.000000
33,-0.01842104,-0.04743945,0.00000047,0.00088137,0.00132210,0.00000007
,-0.00002588,-0.00044560,-0.00000042,-0.00015053,-0.00002473,0.0000002
4,0.00009790,-0.00172705,0.00000008,0.25975682,0.00145617,0.00044965,0
.00000005,0.00113484,-0.00040924,-0.00000016,-0.00187236,0.00017052,0.
,-0.28782778,-0.63279148,-0.00000034,-0.01954393,-0.04968866,-0.000000
21,-0.02976908,-0.00573234,0.00000061,0.00152493,0.00244122,0.00000013
,-0.00000896,-0.00047338,-0.00000072,-0.00057589,-0.00027173,0.0000004
4,-0.00172704,-0.00340395,0.00000012,0.33928963,0.69265820,0.,0.,0.000
46328,0.,0.,-0.00039070,0.,0.00000002,-0.00043781,-0.00000008,0.000000
05,-0.05831432,-0.00000001,0.,0.01938985,0.00000007,-0.00000003,0.0194
9848,0.00000013,-0.00000015,-0.00004059,-0.00000009,0.00000018,-0.0000

0901,0.,0.00000001,-0.00001152,0.,-0.00000001,0.00002764,0.00000003,-0
.00000004,0.01980215,0.00007131,0.00039100,0.00000004,0.00012566,0.000
00220,-0.00000015,-0.00005997,0.00008023,0.00000002,-0.00130579,0.0013
4465,-0.00000029,0.00080506,-0.00107369,-0.00000014,-0.00015294,0.0004
7216,0.00000050,-0.30483518,-0.31253419,0.00000011,0.02391180,-0.00599
069,-0.00000060,-0.02520270,-0.04785234,0.00000037,-0.00010233,-0.0003
6182,0.00000010,-0.00041432,-0.00208053,-0.00000004,0.30715939,0.00031
222,0.00062075,0.00000007,0.00016393,0.00002479,-0.00000023,-0.0001560
4,0.00014008,0.,0.00142015,0.00031238,-0.00000050,0.00095170,-0.000507
20,-0.00000030,-0.00160500,0.00042135,0.00000090,-0.31247145,-0.597701
64,0.00000019,-0.02488371,-0.05046883,-0.00000105,-0.02906065,-0.00130
968,0.00000065,-0.00024975,-0.00060371,0.00000017,-0.00202442,-0.00294
880,-0.00000005,0.36760301,0.65202052,0.00000008,0.00000016,-0.0000131
5,0.00000001,-0.00000004,-0.00001052,-0.00000007,-0.00000003,-0.000010
60,-0.00000010,-0.00000013,0.00041372,0.,0.00000002,-0.00039435,0.0000
0001,0.,-0.00041840,-0.00000010,-0.00000024,-0.05781028,0.,0.00000005,
0.01922505,0.,0.00000002,0.01928033,-0.00000002,-0.00000009,0.00001988
,0.00000009,0.00000011,0.00002254,0.00000009,0.00000016,0.01969577||-0
.00000749,0.00001770,0.,-0.00004535,-0.00003297,0.,-0.00000049,0.00000
023,0.,-0.00003821,0.00005961,0.,-0.00000696,0.00000572,0.,-0.00000113
,0.00004057,0.,0.00000404,0.00006819,0.,0.00000718,-0.00000866,0.,-0.0
0001143,0.00000282,0.,0.00000135,-0.00002278,0.,0.00009875,0.00000929,
0.,-0.00000027,-0.00013973,0.|||@

THERE IS SOMETHING FASCINATING ABOUT SCIENCE.
ONE GETS SUCH WHOLESALE CONJECTURE OUT OF SUCH TRIFLING INVESTMENTS.

-- MARK TWAIN

Job cpu time: 0 days 0 hours 4 minutes 47.0 seconds.
File lengths (MBytes): RWF=   36 Int=   0 D2E=   0 Chk=   5 Scr=   1
Normal termination of Gaussian 98.
Link1: Proceeding to internal job step number 3.

#N Geom=AllCheck Guess=TCheck CCSD(T)/6-31+G(d')

1/29=7,38=1/1;
2/40=1/2;
3/5=11,6=6,7=11,11=9,25=1,30=1/1,2,3;
4/5=101/1;
5/5=2/2;
8/6=7,9=120000,10=1,27=262144000/1,4;
9/5=7,14=2,27=262144000/13;
6/7=2,8=2,9=2,10=2/1;
99/5=1,9=1/99;

Title Card Required

Redundant internal coordinates taken from checkpoint file:
C:\Users\hp\Desktop\3_cbsqb3.chk
Charge = 0 Multiplicity = 1
C,0,1.5637698791,3.4284420444,0.
H,0,2.2282278702,2.5422482383,0.
H,0,0.481755476,3.1913956349,0.
C,0,-0.0820898157,-0.5386793693,0.
H,0,0.4497309692,-1.5086906652,0.
H,0,-1.1860533013,-0.6116939792,0.
C,0,-2.2018717885,-4.2904312843,0.
H,0,-1.7248430438,-5.2905769429,0.
H,0,-3.3099473356,-4.2832988636,0.
O,0,1.9826278561,4.5555092219,0.
O,0,0.4971437781,0.5163517725,0.
O,0,-1.5569866697,-3.2762824654,0.
Recover connectivity data from disk.

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.563770	3.428442	0.000000
2	1	0	2.228228	2.542248	0.000000
3	1	0	0.481755	3.191396	0.000000
4	6	0	-0.082090	-0.538679	0.000000
5	1	0	0.449731	-1.508691	0.000000

6	1	0	-1.186053	-0.611694	0.000000
7	6	0	-2.201872	-4.290431	0.000000
8	1	0	-1.724843	-5.290577	0.000000
9	1	0	-3.309947	-4.283299	0.000000
10	8	0	1.982628	4.555509	0.000000
11	8	0	0.497144	0.516352	0.000000
12	8	0	-1.556987	-3.276282	0.000000

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	H	1.107630	0.000000			
3	H	1.107676	1.863212	0.000000		
4	C	4.294986	3.850933	3.772450	0.000000	
5	H	5.061261	4.424156	4.700195	1.106235	0.000000
6	H	4.887149	4.648082	4.152719	1.106375	1.865581
7	C	8.588426	8.143175	7.948559	4.309190	3.843056
8	H	9.318598	8.773820	8.764299	5.027839	4.362503
9	H	9.122723	8.789737	8.381412	4.943808	4.672647
10	O	1.202382	2.028186	2.028158	5.496710	6.254941
11	O	3.101284	2.664753	2.675088	1.203579	2.025597
12	O	7.395435	6.941408	6.781396	3.109629	2.674191

		6	7	8	9	10
6	H	0.000000				
7	C	3.816411	0.000000			
8	H	4.709803	1.108083	0.000000		
9	H	4.241652	1.108099	1.878075	0.000000	
10	O	6.061397	9.785740	10.520967	10.302227	0.000000
11	O	2.026238	5.512699	6.217527	6.126221	4.303656
12	O	2.690283	1.201821	2.021276	2.021621	8.594523

		11	12
11	O	0.000000	
12	O	4.313181	0.000000

Interatomic angles:

H2-C1-H3=114.5051 H5-C4-H6=114.9504 H8-C7-H9=115.868
H2-C1-O10=122.751 H3-C1-O10=122.7439 H2-H3-O10= 62.6567
C1-H2-O11=102.6247 C1-H3-O11=102.0275 H3-H2-O11= 69.8765
H2-O11-C4=168.2545 H3-O11-C4=150.9027 H2-O11-H5=140.8281
H3-O11-H5=178.3292 H5-C4-O11=122.498 H2-O11-H6=164.3424
H3-O11-H6=123.4996 H6-C4-O11=122.5516 H6-H5-O11= 62.6027
O10-H2-O11=132.5316 O10-H3-O11=131.9375 C4-H5-O12=102.6405
C4-H6-O12=101.7091 H6-H5-O12= 70.1134 H5-O12-C7=163.8266
H6-O12-C7=155.4733 H5-O12-H8=136.1384 H6-O12-H8=176.8385
H8-C7-O12=122.049 H5-O12-H9=168.5011 H6-O12-H9=127.801
H9-C7-O12=122.083 H9-H8-O12= 62.3291 O11-H5-O12=132.716
O11-H6-O12=131.7543

Stoichiometry C3H6O3
Framework group CS[SG(C3H6O3)]
Deg. of freedom 21
Full point group CS NOp 2
Largest Abelian subgroup CS NOp 2
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.029422	-3.624897	0.000000
2	1	0	-1.819803	-2.848919	0.000000
3	1	0	0.004532	-3.227549	0.000000
4	6	0	0.000000	0.544898	0.000000
5	1	0	-0.671885	1.423719	0.000000
6	1	0	1.080364	0.783394	0.000000
7	6	0	1.530381	4.573180	0.000000
8	1	0	0.908123	5.490046	0.000000
9	1	0	2.626885	4.733062	0.000000
10	8	0	-1.273705	-4.802203	0.000000
11	8	0	-0.413681	-0.585354	0.000000
12	8	0	1.045639	3.473453	0.000000

Rotational constants (GHZ): 70.1259093 0.4410420 0.4382855
Isotopes: C-12,H-1,H-1,C-12,H-1,H-1,C-12,H-1,H-1,O-16,O-16,O-16
Standard basis: 6-31+(d') (6D, 7F)
There are 96 symmetry adapted basis functions of A' symmetry.

```
There are    30 symmetry adapted basis functions of A"  symmetry.
Crude estimate of integral set expansion from redundant integrals=1.000.
Integral buffers will be    262144 words long.
Raffenetti 1 integral format.
Two-electron integral symmetry is turned on.
  126 basis functions      216 primitive gaussians
   24 alpha electrons       24 beta electrons
     nuclear repulsion energy       175.9786698479 Hartrees.
One-electron integrals computed using PRISM.
NBasis=   126 RedAO= T  NBF=    96    30
NBsUse=   126 1.00D-04 NBFU=    96    30
Initial guess read from the checkpoint file:
C:\Users\hp\Desktop\3_cbsqb3.chk
Unable to project full set of read-in orbitals.
Projecting just the  24 occupied ones.
Initial guess orbital symmetries:
     Occupied  (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A') (A') (A') (A") (A")
               (A") (A') (A') (A')
     Virtual   (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A") (A") (A") (A") (A")
               (A") (A") (A") (A") (A") (A") (A") (A") (A") (A")
               (A") (A") (A") (A") (A") (A") (A") (A") (A") (A")
               (A") (A")
Requested convergence on RMS density matrix=1.00D-08 within  64 cycles.
Requested convergence on MAX density matrix=1.00D-06.
SCF Done:  E(RHF) =  -341.621947434     A.U. after   11 cycles
          Convg  =    0.7702D-08           -V/T =  2.0027
          S**2   =   0.0000
Range of M.O.s used for correlation:    7   126
NBasis=   126 NAE=    24 NBE=    24 NFC=     6 NFV=     0
NROrb=    120 NOA=    18 NOB=    18 NVA=   102 NVB=   102
Estimate disk for full transformation   142681198 words.
Semi-Direct transformation.
ModeAB=          4 MOrb=          69 LenV=      5926400
LASXX=     21693051 LTotXX=    28950729 LenRXX=    36666843
LTotAB=     7716114 MaxLAS=    47139180 LenRXY=          0
NonZer=    51102216 LenScr=    82518016 LnRSAI=    53762040
LnScr1=    86481920 LExtra=    1204881 Total=    260633700
MaxDsk=   262144000 SrtSym=          T ITran=           5
JobTyp=0 Pass  1:  I=   1 to  60.
JobTyp=0 Pass  2:  I=  61 to 120.
Spin components of T(2) and E(2):
   alpha-alpha T2 =       0.3623437644D-01 E2=     -0.1199163840D+00
   alpha-beta  T2 =       0.2172259971D+00 E2=     -0.7019070678D+00
   beta-beta   T2 =       0.3623437644D-01 E2=     -0.1199163840D+00
ANorm=    0.1135647282D+01
E2=      -0.9417398358D+00 EUMP2=      -0.34256368726964D+03
Iterations=  50 Convergence= 0.100D-06
Iteration Nr.   1
**********************
MP4(R+Q)=  0.13854665D-01
E3=      -0.13969225D-01       EUMP3=     -0.34257765649D+03
E4(DQ)=   -0.12180831D-01       UMP4(DQ)=   -0.34258983733D+03
E4(SDQ)=  -0.27077965D-01       UMP4(SDQ)=  -0.34260473446D+03
DE(CORR)= -0.94083117D+00       E(CORR)=    -0.34256277860D+03
NORM(A)=   0.11421767D+01
Iteration Nr.   2
**********************
DE(CORR)= -0.97441233D+00       E(CORR)=    -0.34259635976D+03
NORM(A)=   0.11585233D+01
Iteration Nr.   3
**********************
DE(CORR)= -0.97695256D+00       E(CORR)=    -0.34259890000D+03
NORM(A)=   0.11637939D+01
Iteration Nr.   4
**********************
DE(CORR)= -0.98052700D+00       E(CORR)=    -0.34260247443D+03
```

```
NORM(A)=   0.11653624D+01
Iteration Nr.  5
**********************
DE(CORR)= -0.98093622D+00      E(CORR)=   -0.34260288366D+03
NORM(A)=   0.11658025D+01
Iteration Nr.  6
**********************
DE(CORR)= -0.98098291D+00      E(CORR)=   -0.34260293034D+03
NORM(A)=   0.11658297D+01
Iteration Nr.  7
**********************
DE(CORR)= -0.98098362D+00      E(CORR)=   -0.34260293105D+03
NORM(A)=   0.11658350D+01
Iteration Nr.  8
**********************
DE(CORR)= -0.98097801D+00      E(CORR)=   -0.34260292544D+03
NORM(A)=   0.11658406D+01
Iteration Nr.  9
**********************
DE(CORR)= -0.98097951D+00      E(CORR)=   -0.34260292694D+03
NORM(A)=   0.11658421D+01
Iteration Nr.  10
**********************
DE(CORR)= -0.98097982D+00      E(CORR)=   -0.34260292726D+03
NORM(A)=   0.11658432D+01
Iteration Nr.  11
**********************
DE(CORR)= -0.98098037D+00      E(CORR)=   -0.34260292780D+03
NORM(A)=   0.11658439D+01
Iteration Nr.  12
**********************
DE(CORR)= -0.98098068D+00      E(CORR)=   -0.34260292811D+03
NORM(A)=   0.11658443D+01
Iteration Nr.  13
**********************
DE(CORR)= -0.98098077D+00      E(CORR)=   -0.34260292820D+03
NORM(A)=   0.11658446D+01
Iteration Nr.  14
**********************
DE(CORR)= -0.98098084D+00      E(CORR)=   -0.34260292827D+03
NORM(A)=   0.11658446D+01
Largest amplitude= 5.43D-02
Time for triples=      548.00 seconds.
T4(CCSD)= -0.34616021D-01
T5(CCSD)=  0.33964442D-02
CCSD(T)= -0.34263414785D+03

**********************************************************************

        Population analysis using the SCF density.

**********************************************************************

Orbital Symmetries:
    Occupied  (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
              (A') (A') (A') (A') (A') (A') (A') (A') (A") (A")
              (A") (A') (A') (A')
    Virtual   (A") (A') (A') (A") (A') (A') (A") (A') (A') (A')
              (A") (A') (A") (A") (A') (A') (A') (A") (A') (A')
              (A') (A') (A") (A') (A') (A') (A') (A") (A') (A')
              (A') (A') (A') (A') (A') (A') (A") (A") (A') (A")
              (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
              (A') (A') (A') (A') (A") (A') (A") (A") (A') (A")
              (A") (A') (A') (A") (A') (A') (A") (A") (A") (A')
              (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
              (A') (A") (A") (A') (A") (A') (A') (A') (A") (A")
              (A') (A") (A') (A') (A') (A') (A') (A') (A') (A')
              (A') (A')
 The electronic state is 1-A'.
Alpha  occ. eigenvalues --  -20.61371 -20.58566 -20.56182 -11.37397 -11.34350
Alpha  occ. eigenvalues --  -11.31901  -1.43977  -1.41132  -1.38696  -0.89492
Alpha  occ. eigenvalues --   -0.86481  -0.83849  -0.71915  -0.68912  -0.68506
Alpha  occ. eigenvalues --   -0.66435  -0.65408  -0.62468  -0.56608  -0.53891
Alpha  occ. eigenvalues --   -0.51369  -0.46806  -0.43865  -0.41202
```

Alpha virt. eigenvalues -- 0.05670 0.06226 0.07722 0.07830 0.08242
Alpha virt. eigenvalues -- 0.09752 0.09787 0.11090 0.12076 0.14581
Alpha virt. eigenvalues -- 0.15784 0.16531 0.18421 0.19787 0.22390
Alpha virt. eigenvalues -- 0.28874 0.29546 0.31485 0.31889 0.32946
Alpha virt. eigenvalues -- 0.33320 0.34689 0.35721 0.36354 0.37309
Alpha virt. eigenvalues -- 0.37582 0.38727 0.39091 0.40729 0.43045
Alpha virt. eigenvalues -- 0.44496 0.45487 0.47901 0.51230 0.65999
Alpha virt. eigenvalues -- 0.68924 0.85102 0.87863 0.89900 0.90329
Alpha virt. eigenvalues -- 0.94328 0.96454 0.97812 0.99615 1.06017
Alpha virt. eigenvalues -- 1.11569 1.12143 1.17205 1.19164 1.19897
Alpha virt. eigenvalues -- 1.22116 1.26633 1.41302 1.43230 1.44355
Alpha virt. eigenvalues -- 1.47191 1.47300 1.47871 1.49276 1.49672
Alpha virt. eigenvalues -- 1.51707 1.51920 1.53218 1.53678 1.54573
Alpha virt. eigenvalues -- 1.60300 1.60656 1.63962 1.66473 1.85284
Alpha virt. eigenvalues -- 1.90844 1.95093 2.01425 2.07873 2.11648
Alpha virt. eigenvalues -- 2.19538 2.23526 2.24810 2.41327 2.46742
Alpha virt. eigenvalues -- 2.47939 3.19032 3.21694 3.22121 3.24255
Alpha virt. eigenvalues -- 3.24882 3.27209 3.54502 3.60950 3.63566
Alpha virt. eigenvalues -- 3.65921 3.66305 3.68585 3.70830 3.72252
Alpha virt. eigenvalues -- 3.75042 4.09986 4.17317 4.23188 6.66054
Alpha virt. eigenvalues -- 6.68994 6.73259

Condensed to atoms (all electrons):

		1	2	3	4	5	6
1	C	4.935365	0.394144	0.393343	-0.001401	-0.000519	0.000249
2	H	0.394144	0.524043	-0.055241	0.000725	0.000010	-0.000009
3	H	0.393343	-0.055241	0.527495	0.001435	-0.000009	0.000031
4	C	-0.001401	0.000725	0.001435	4.979475	0.405915	0.397725
5	H	-0.000519	0.000010	-0.000009	0.405915	0.512179	-0.051692
6	H	0.000249	-0.000009	0.000031	0.397725	-0.051692	0.513874
7	C	-0.000002	0.000001	0.000001	-0.003917	0.000259	0.000150
8	H	0.000000	0.000000	0.000000	-0.000439	0.000016	-0.000010
9	H	0.000000	0.000000	0.000000	0.000048	-0.000010	0.000025
10	O	0.387054	-0.055897	-0.056696	0.000488	0.000000	0.000000
11	O	-0.000948	-0.002906	-0.003934	0.325467	-0.065620	-0.058007
12	O	0.000017	0.000000	0.000000	0.007524	-0.002483	-0.003238

		7	8	9	10	11	12
1	C	-0.000002	0.000000	0.000000	0.387054	-0.000948	0.000017
2	H	0.000001	0.000000	0.000000	-0.055897	-0.002906	0.000000
3	H	0.000001	0.000000	0.000000	-0.056696	-0.003934	0.000000
4	C	-0.003917	-0.000439	0.000048	0.000488	0.325467	0.007524
5	H	0.000259	0.000016	-0.000010	0.000000	-0.065620	-0.002483
6	H	0.000150	-0.000010	0.000025	0.000000	-0.058007	-0.003238
7	C	4.965349	0.398384	0.393353	0.000000	0.000181	0.330236
8	H	0.398384	0.527902	-0.055759	0.000000	-0.000002	-0.064096
9	H	0.393353	-0.055759	0.527937	0.000000	0.000000	-0.059521
10	O	0.000000	0.000000	0.000000	8.022193	-0.000109	0.000000
11	O	0.000181	-0.000002	0.000000	-0.000109	8.101382	0.000246
12	O	0.330236	-0.064096	-0.059521	0.000000	0.000246	8.073682

Total atomic charges:

		1
1	C	-0.107303
2	H	0.195131
3	H	0.193574
4	C	-0.113045
5	H	0.201955
6	H	0.200901
7	C	-0.083995
8	H	0.194005
9	H	0.193927
10	O	-0.297034
11	O	-0.295750
12	O	-0.282368

Sum of Mulliken charges= 0.00000

Atomic charges with hydrogens summed into heavy atoms:

		1
1	C	0.281402
2	H	0.000000
3	H	0.000000
4	C	0.289812
5	H	0.000000
6	H	0.000000
7	C	0.303937
8	H	0.000000
9	H	0.000000

10 O   -0.297034
11 O   -0.295750
12 O   -0.282368
Sum of Mulliken charges=   0.00000
Electronic spatial extent (au): <R**2>= 2292.7486
Charge=   0.0000 electrons
Dipole moment (Debye):
   X=   3.1043   Y=   9.3642   Z=   0.0000 Tot=   9.8653
Quadrupole moment (Debye-Ang):
  XX=   -33.3380   YY=   -38.4301   ZZ=   -35.3628
  XY=   1.6538   XZ=   0.0000   YZ=   0.0000
Octapole moment (Debye-Ang**2):
 XXX=   12.0767 YYY=   314.0223 ZZZ=   0.0000 XYY=   91.8964
 XXY=   31.2562 XXZ=   0.0000 XZZ=   -0.1845 YZZ=   -0.4757
 YYZ=   0.0000 XYZ=   0.0000
Hexadecapole moment (Debye-Ang**3):
XXXX= -263.6739 YYYY= -2688.0357 ZZZZ=   -31.5713 XXXY= -344.7838
XXXZ=   0.0000 YYYX= -352.0720 YYYZ=   0.0000 ZZZX=   0.0000
ZZZY=   0.0000 XXYY= -433.3324 XXZZ=   -52.6413 YYZZ= -426.0743
XXYZ=   0.0000 YYXZ=   0.0000 ZZXY= -123.0505
N-N= 1.759786698479D+02 E-N=-1.156695623047D+03 KE= 3.407099869021D+02
Symmetry A'   KE= 3.302005094644D+02
Symmetry A"   KE= 1.050947743761D+01
1|1|UNPC-UNK|SP|RCCSD(T)-FC|6-31+(d')|C3H6O3|PCUSER|11-Oct-2015|0||#N
GEOM=ALLCHECK GUESS=TCHECK CCSD(T)/6-31+G(D')||Title Card Required||0,
1|C,1.5637698791,3.4284420444,0.|H,2.2282278702,2.5422482383,0.|H,0.48
1755476,3.1913956349,0.|C,-0.0820898157,-0.5386793693,0.|H,0.449730969
2,-1.5086906652,0.|H,-1.1860533013,-0.6116939792,0.|C,-2.2018717885,-4
.2904312843,0.|H,-1.7248430438,-5.2905769429,0.|H,-3.3099473356,-4.283
2988636,0.|O,1.9826278561,4.5555092219,0.|O,0.4971437781,0.5163517725,
0.|O,-1.5569866697,-3.2762824654,0.||Version=x86-Win32-G98RevA.11.4|St
ate=1-A'|HF=-341.6219474|MP2=-342.5636873|MP3=-342.5776565|MP4D=-342.6
03692|MP4DQ=-342.5898373|MP4SDQ=-342.6047345|CCSD=-342.6029283|CCSD(T)
=-342.6341479|RMSD=7.702e-009|PG=CS [SG(C3H6O3)]||@

... I FELL INTO A REVERIE ... THE ATOMS WERE GAMBOLING BEFORE MY EYES
... I SAW HOW TWO SMALL ONES UNITED TO FORM A PAIR;
HOW THE LARGER ONES SEIZED TWO OF THE SMALLER ONES;
HOW STILL LARGER ONES KEPT HOLD OF THREE OR FOUR
SMALLER ONES ... I SAW HOW THE LARGER ONES FORMED A CHAIN ...
THIS WAS THE ORIGIN OF THE STRUCTURE THEORY.

                          -- C.F.KEKULE VON STRADONITZ
Job cpu time: 0 days 0 hours 24 minutes 37.0 seconds.
File lengths (MBytes): RWF= 1993 Int=   0 D2E=   0 Chk=   5 Scr=   1
Normal termination of Gaussian 98.
Link1: Proceeding to internal job step number 4.

#N Geom=AllCheck Guess=TCheck MP4SDQ/CBSB4

1/29=7,38=1/1;
2/40=1/2;
3/5=13,11=9,25=1,30=1/1,2,3;
4/5=101/1;
5/5=2/2;
8/6=3,9=120000,10=1,27=262144000/1,4;
9/5=4,27=262144000/13;
6/7=2,8=2,9=2,10=2/1;
99/5=1,9=1/99;

Title Card Required

Redundant internal coordinates taken from checkpoint file:
C:\Users\hp\Desktop\3_cbsqb3.chk
Charge = 0 Multiplicity = 1
C,0,1.5637698791,3.4284420444,0.
H,0,2.2282278702,2.5422482383,0.
H,0,0.481755476,3.1913956349,0.
C,0,-0.0820898157,-0.5386793693,0.
H,0,0.4497309692,-1.5086906652,0.
H,0,-1.1860533013,-0.6116939792,0.
C,0,-2.2018717885,-4.2904312843,0.
H,0,-1.7248430438,-5.2905769429,0.

H,0,-3.3099473356,-4.2832988636,0.
O,0,1.9826278561,4.5555092219,0.
O,0,0.4971437781,0.5163517725,0.
O,0,-1.5569866697,-3.2762824654,0.
Recover connectivity data from disk.

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.563770	3.428442	0.000000
2	1	0	2.228228	2.542248	0.000000
3	1	0	0.481755	3.191396	0.000000
4	6	0	-0.082090	-0.538679	0.000000
5	1	0	0.449731	-1.508691	0.000000
6	1	0	-1.186053	-0.611694	0.000000
7	6	0	-2.201872	-4.290431	0.000000
8	1	0	-1.724843	-5.290577	0.000000
9	1	0	-3.309947	-4.283299	0.000000
10	8	0	1.982628	4.555509	0.000000
11	8	0	0.497144	0.516352	0.000000
12	8	0	-1.556987	-3.276282	0.000000

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	H	1.107630	0.000000			
3	H	1.107676	1.863212	0.000000		
4	C	4.294986	3.850933	3.772450	0.000000	
5	H	5.061261	4.424156	4.700195	1.106235	0.000000
6	H	4.887149	4.648082	4.152719	1.106375	1.865581
7	C	8.588426	8.143175	7.948559	4.309190	3.843056
8	H	9.318598	8.773820	8.764299	5.027839	4.362503
9	H	9.122723	8.789737	8.381412	4.943808	4.672647
10	O	1.202382	2.028186	2.028158	5.496710	6.254941
11	O	3.101284	2.664753	2.675088	1.203579	2.025597
12	O	7.395435	6.941408	6.781396	3.109629	2.674191

		6	7	8	9	10
6	H	0.000000				
7	C	3.816411	0.000000			
8	H	4.709803	1.108083	0.000000		
9	H	4.241652	1.108099	1.878075	0.000000	
10	O	6.061397	9.785740	10.520967	10.302227	0.000000
11	O	2.026238	5.512699	6.217527	6.126221	4.303656
12	O	2.690283	1.201821	2.021276	2.021621	8.594523

		11	12
11	O	0.000000	
12	O	4.313181	0.000000

Interatomic angles:

H2-C1-H3=114.5051 H5-C4-H6=114.9504 H8-C7-H9=115.868
H2-C1-O10=122.751 H3-C1-O10=122.7439 H2-H3-O10= 62.6567
C1-H2-O11=102.6247 C1-H3-O11=102.0275 H3-H2-O11= 69.8765
H2-O11-C4=168.2545 H3-O11-C4=150.9027 H2-O11-H5=140.8281
H3-O11-H5=178.3292 H5-C4-O11=122.498 H2-O11-H6=164.3424
H3-O11-H6=123.4996 H6-C4-O11=122.5516 H6-H5-O11= 62.6027
O10-H2-O11=132.5316 O10-H3-O11=131.9375 C4-H5-O12=102.6405
C4-H6-O12=101.7091 H6-H5-O12= 70.1134 H5-O12-C7=163.8266
H6-O12-C7=155.4733 H5-O12-H8=136.1384 H6-O12-H8=176.8385
H8-C7-O12=122.049 H5-O12-H9=168.5011 H6-O12-H9=127.801
H9-C7-O12=122.083 H9-H8-O12= 62.3291 O11-H5-O12=132.716
O11-H6-O12=131.7543

Stoichiometry C3H6O3
Framework group CS[SG(C3H6O3)]
Deg. of freedom 21
Full point group CS NOp 2
Largest Abelian subgroup CS NOp 2
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.029422	-3.624897	0.000000
2	1	0	-1.819803	-2.848919	0.000000

```
  3        1           0       0.004532   -3.227549    0.000000
  4        6           0       0.000000    0.544898    0.000000
  5        1           0      -0.671885    1.423719    0.000000
  6        1           0       1.080364    0.783394    0.000000
  7        6           0       1.530381    4.573180    0.000000
  8        1           0       0.908123    5.490046    0.000000
  9        1           0       2.626885    4.733062    0.000000
 10        8           0      -1.273705   -4.802203    0.000000
 11        8           0      -0.413681   -0.585354    0.000000
 12        8           0       1.045639    3.473453    0.000000
---------------------------------------------------------------------
Rotational constants (GHZ):     70.1259093      0.4410420      0.4382855
Isotopes: C-12,H-1,H-1,C-12,H-1,H-1,C-12,H-1,H-1,O-16,O-16,O-16
Standard basis: CBSB4 (6D, 7F)
There are   108 symmetry adapted basis functions of A'  symmetry.
There are    36 symmetry adapted basis functions of A"  symmetry.
Crude estimate of integral set expansion from redundant integrals=1.000.
Integral buffers will be    262144 words long.
Raffenetti 1 integral format.
Two-electron integral symmetry is turned on.
  144 basis functions      234 primitive gaussians
   24 alpha electrons       24 beta electrons
      nuclear repulsion energy       175.9786698479 Hartrees.
One-electron integrals computed using PRISM.
NBasis=   144 RedAO= T  NBF=   108    36
NBsUse=   144 1.00D-04 NBFU=   108    36
Initial guess read from the checkpoint file:
C:\Users\hp\Desktop\3_cbsqb3.chk
Initial guess orbital symmetries:
     Occupied  (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A') (A') (A") (A")
               (A") (A') (A') (A')
     Virtual   (A") (A') (A') (A") (A') (A') (A") (A') (A') (A')
               (A") (A') (A") (A") (A') (A') (A') (A") (A') (A')
               (A') (A') (A") (A') (A') (A') (A') (A") (A') (A')
               (A') (A') (A') (A') (A') (A') (A") (A") (A') (A")
               (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
               (A') (A') (A') (A') (A") (A') (A") (A") (A') (A")
               (A") (A') (A') (A") (A') (A') (A") (A") (A") (A')
               (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
               (A') (A") (A") (A') (A") (A') (A') (A') (A") (A")
               (A') (A") (A') (A') (A') (A') (A') (A') (A') (A')
               (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
               (A') (A') (A') (A') (A") (A") (A") (A") (A") (A")
Requested convergence on RMS density matrix=1.00D-08 within  64 cycles.
Requested convergence on MAX density matrix=1.00D-06.
SCF Done:  E(RHF) =  -341.631268509     A.U. after   10 cycles
          Convg  =    0.2953D-08             -V/T =  2.0026
          S**2   =   0.0000
Range of M.O.s used for correlation:     7   144
NBasis=   144 NAE=    24 NBE=    24 NFC=     6 NFV=     0
NROrb=    138 NOA=    18 NOB=    18 NVA=   120 NVB=   120
Semi-Direct transformation.
ModeAB=          4 MOrb=          18 LenV=      5851734
LASXX=     3325572 LTotXX=     3325572 LenRXX=     6779358
LTotAB=     3453786 MaxLAS=     20324088 LenRXY=          0
NonZer=    10104930 LenScr=    17172992 LnRSAI=    20324088
LnScr1=    36188160 LExtra=     1495332 Total=     81959930
MaxDsk=   262144000 SrtSym=          T ITran=          3
JobTyp=0 Pass  1:  I=   1 to  18.
Spin components of T(2) and E(2):
   alpha-alpha T2 =       0.3675740612D-01 E2=     -0.1217664631D+00
   alpha-beta  T2 =       0.2254098544D+00 E2=     -0.7358116963D+00
   beta-beta   T2 =       0.3675740612D-01 E2=     -0.1217664631D+00
ANorm=    0.1139703763D+01
E2=      -0.9793446224D+00 EUMP2=      -0.34261061313117D+03
Would need an additional   104226454 words for in-memory AO integral storage.
DD1Dir will call FoFDir   2 times, MxPair=       172
NAB=   171 NAA=     0 NBB=     0 NumPrc=  1.
Petite list used in FoFDir.
MinBra= 0 MaxBra= 2 Meth= 1.
IRaf=       0 NMat= 172 IRICut=     172 DoRegI=T DoRafI=T ISym2E=-1 JSym2E=1.
MP4(R+Q)=  0.15338613D-01
E3=      -0.18233162D-01       EUMP3=      -0.34262884629D+03
```

E4(DQ)= -0.11436769D-01 UMP4(DQ)= -0.34264028306D+03
E4(SDQ)= -0.26499876D-01 UMP4(SDQ)= -0.34265534617D+03
Largest amplitude= 4.19D-02

****

Population analysis using the SCF density.

****

Orbital Symmetries:
Occupied (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
(A') (A') (A') (A') (A') (A') (A') (A') (A") (A")
(A") (A') (A') (A')
Virtual (A") (A') (A') (A") (A') (A') (A") (A') (A') (A')
(A") (A') (A") (A") (A') (A') (A') (A") (A') (A')
(A') (A') (A") (A') (A') (A') (A') (A") (A') (A')
(A') (A') (A') (A') (A') (A') (A") (A") (A') (A")
(A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
(A') (A") (A") (A') (A") (A') (A') (A") (A') (A')
(A") (A") (A") (A') (A') (A') (A") (A") (A') (A')
(A') (A') (A') (A') (A') (A') (A') (A') (A") (A")
(A") (A") (A') (A") (A') (A") (A') (A') (A') (A')
(A') (A') (A') (A') (A') (A') (A') (A') (A') (A")
(A") (A") (A') (A') (A') (A") (A") (A") (A') (A')
(A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
The electronic state is 1-A'.
Alpha occ. eigenvalues -- -20.61373 -20.58552 -20.56153 -11.37398 -11.34342
Alpha occ. eigenvalues -- -11.31895 -1.43966 -1.41108 -1.38662 -0.89469
Alpha occ. eigenvalues -- -0.86457 -0.83814 -0.71846 -0.68828 -0.68462
Alpha occ. eigenvalues -- -0.66342 -0.65354 -0.62404 -0.56587 -0.53858
Alpha occ. eigenvalues -- -0.51325 -0.46749 -0.43799 -0.41127
Alpha virt. eigenvalues -- 0.05611 0.06175 0.07698 0.07778 0.08174
Alpha virt. eigenvalues -- 0.09738 0.09739 0.11021 0.12072 0.14505
Alpha virt. eigenvalues -- 0.15757 0.16501 0.18399 0.19791 0.22345
Alpha virt. eigenvalues -- 0.28844 0.29500 0.31473 0.31847 0.32906
Alpha virt. eigenvalues -- 0.33284 0.34590 0.35709 0.36314 0.37194
Alpha virt. eigenvalues -- 0.37509 0.38501 0.39077 0.40660 0.42980
Alpha virt. eigenvalues -- 0.44462 0.45461 0.47906 0.51205 0.65919
Alpha virt. eigenvalues -- 0.68847 0.85109 0.87859 0.89518 0.90321
Alpha virt. eigenvalues -- 0.91775 0.94677 0.96579 0.98612 1.03435
Alpha virt. eigenvalues -- 1.05533 1.05550 1.11266 1.13331 1.15567
Alpha virt. eigenvalues -- 1.15830 1.21767 1.25023 1.25860 1.27356
Alpha virt. eigenvalues -- 1.40182 1.42470 1.46458 1.46964 1.48701
Alpha virt. eigenvalues -- 1.49135 1.50505 1.50653 1.51443 1.52060
Alpha virt. eigenvalues -- 1.54410 1.54853 1.57838 1.59850 1.72505
Alpha virt. eigenvalues -- 1.77447 1.79844 1.80494 1.81077 1.85733
Alpha virt. eigenvalues -- 1.89137 1.95045 1.97854 2.00489 2.04259
Alpha virt. eigenvalues -- 2.06639 2.08831 2.09950 2.11627 2.13267
Alpha virt. eigenvalues -- 2.13617 2.14989 2.15822 2.17412 2.23620
Alpha virt. eigenvalues -- 2.66534 2.71328 2.73614 2.82348 2.83388
Alpha virt. eigenvalues -- 2.85662 2.87138 2.88853 2.92045 3.22291
Alpha virt. eigenvalues -- 3.24933 3.27484 3.29884 3.32400 3.34426
Alpha virt. eigenvalues -- 3.62222 3.64945 3.67736 3.72822 3.86086
Alpha virt. eigenvalues -- 3.89512 3.92041 3.95226 3.97661 4.12329
Alpha virt. eigenvalues -- 4.20344 4.25859 6.71508 6.74155 6.77797
Condensed to atoms (all electrons):

		1	2	3	4	5	6
1	C	4.661558	0.421148	0.419640	-0.001410	-0.000732	0.000061
2	H	0.421148	0.597581	-0.058247	0.001096	0.000007	-0.000011
3	H	0.419640	-0.058247	0.600444	0.002038	-0.000009	0.000029
4	C	-0.001410	0.001096	0.002038	4.718985	0.437857	0.429451
5	H	-0.000732	0.000007	-0.000009	0.437857	0.585196	-0.054100
6	H	0.000061	-0.000011	0.000029	0.429451	-0.054100	0.586816
7	C	-0.000006	0.000002	0.000002	-0.004803	0.000251	0.000295
8	H	0.000000	0.000000	0.000000	-0.000665	0.000012	-0.000010
9	H	0.000000	0.000000	0.000000	-0.000174	-0.000012	0.000022
10	O	0.395008	-0.057484	-0.058492	0.000441	0.000001	0.000001
11	O	-0.003247	-0.005253	-0.006050	0.323485	-0.071531	-0.064064
12	O	0.000024	0.000001	0.000001	0.005845	-0.004244	-0.005003

		7	8	9	10	11	12
1	C	-0.000006	0.000000	0.000000	0.395008	-0.003247	0.000024
2	H	0.000002	0.000000	0.000000	-0.057484	-0.005253	0.000001
3	H	0.000002	0.000000	0.000000	-0.058492	-0.006050	0.000001

```
 4  C   -0.004803  -0.000665  -0.000174   0.000441   0.323485   0.005845
 5  H    0.000251   0.000012  -0.000012   0.000001  -0.071531  -0.004244
 6  H    0.000295  -0.000010   0.000022   0.000001  -0.064064  -0.005003
 7  C    4.727354   0.429373   0.424451   0.000000   0.000247   0.320640
 8  H    0.429373   0.597405  -0.058126   0.000000  -0.000001  -0.070904
 9  H    0.424451  -0.058126   0.597572   0.000000   0.000000  -0.066434
10  O    0.000000   0.000000   0.000000   8.048980  -0.000194   0.000000
11  O    0.000247  -0.000001   0.000000  -0.000194   8.133571   0.000330
12  O    0.320640  -0.070904  -0.066434   0.000000   0.000330   8.103438
Total atomic charges:
             1
 1  C    0.107957
 2  H    0.101161
 3  H    0.100645
 4  C    0.087855
 5  H    0.107305
 6  H    0.106514
 7  C    0.102194
 8  H    0.102915
 9  H    0.102701
10  O   -0.328262
11  O   -0.307293
12  O   -0.283692
Sum of Mulliken charges=   0.00000
Atomic charges with hydrogens summed into heavy atoms:
             1
 1  C    0.309763
 2  H    0.000000
 3  H    0.000000
 4  C    0.301673
 5  H    0.000000
 6  H    0.000000
 7  C    0.307810
 8  H    0.000000
 9  H    0.000000
10  O   -0.328262
11  O   -0.307293
12  O   -0.283692
Sum of Mulliken charges=   0.00000
Electronic spatial extent (au):  <R**2>=  2292.7450
Charge=     0.0000 electrons
Dipole moment (Debye):
   X=     3.1088    Y=     9.3814    Z=     0.0000  Tot=     9.8831
Quadrupole moment (Debye-Ang):
  XX=   -33.3301   YY=   -38.5089   ZZ=   -35.2870
  XY=     1.6201   XZ=     0.0000   YZ=     0.0000
Octapole moment (Debye-Ang**2):
 XXX=    12.1849  YYY=   314.1840  ZZZ=     0.0000  XYY=    91.7903
 XXY=    31.3253  XXZ=     0.0000  XZZ=    -0.1744  YZZ=    -0.4465
 YYZ=     0.0000  XYZ=     0.0000
Hexadecapole moment (Debye-Ang**3):
XXXX=  -263.7097 YYYY= -2692.1511 ZZZZ=   -31.3529 XXXY=  -344.5847
XXXZ=     0.0000 YYYX=  -354.0611 YYYZ=     0.0000 ZZZX=     0.0000
ZZZY=     0.0000 XXYY=  -433.7837 XXZZ=   -52.6324 YYZZ=  -425.2725
XXYZ=     0.0000 YYXZ=     0.0000 ZZXY=  -122.7795
N-N= 1.759786698479D+02 E-N=-1.156758169928D+03  KE= 3.407356844662D+02
Symmetry A'   KE= 3.302336667576D+02
Symmetry A"   KE= 1.050201770859D+01
1|1|UNPC-UNK|SP|RMP4SDQ-FC|CBSB4|C3H6O3|PCUSER|11-Oct-2015|0||#N GEOM=
ALLCHECK GUESS=TCHECK MP4SDQ/CBSB4||Title Card Required||0,1|C,1.56376
98791,3.4284420444,0.|H,2.2282278702,2.5422482383,0.|H,0.481755476,3.1
913956349,0.|C,-0.0820898157,-0.5386793693,0.|H,0.4497309692,-1.508690
6652,0.|H,-1.1860533013,-0.6116939792,0.|C,-2.2018717885,-4.2904312843
,0.|H,-1.7248430438,-5.2905769429,0.|H,-3.3099473356,-4.2832988636,0.|
O,1.9826278561,4.5555092219,0.|O,0.4971437781,0.5163517725,0.|O,-1.556
9866697,-3.2762824654,0.||Version=x86-Win32-G98RevA.11.4|State=1-A'|HF
=-341.6312685|MP2=-342.6106131|MP3=-342.6288463|MP4D=-342.6556217|MP4D
Q=-342.6402831|MP4SDQ=-342.6553462|RMSD=2.953e-009|PG=CS [SG(C3H6O3)]|
|@
```

SCIENCE SANS CONSCIENCE N'EST QUE RUINE DE L'AME.

-- RABELAIS

Job cpu time: 0 days 0 hours 2 minutes 18.0 seconds.
File lengths (MBytes): RWF= 1993 Int= 0 D2E= 0 Chk= 5 Scr= 1
Normal termination of Gaussian 98.
Link1: Proceeding to internal job step number 5.

#N Geom=AllCheck Guess=TCheck MP2/CBSB3 CBSExtrap=(NMin=10,MinPop)

1/29=7,38=1/1;
2/40=1/2;
3/5=12,11=9,25=1,30=1/1,2,3;
4/5=101/1;
5/5=2/2;
8/10=1,27=262144000,41=10,43=4/1,4,3;
6/7=2,8=2,9=2,10=2/1;
99/5=1,9=1/99;

Title Card Required

Redundant internal coordinates taken from checkpoint file:
C:\Users\hp\Desktop\3_cbsqb3.chk
Charge = 0 Multiplicity = 1
C,0,1.5637698791,3.4284420444,0.
H,0,2.2282278702,2.5422482383,0.
H,0,0.481755476,3.1913956349,0.
C,0,-0.0820898157,-0.5386793693,0.
H,0,0.4497309692,-1.5086906652,0.
H,0,-1.1860533013,-0.6116939792,0.
C,0,-2.2018717885,-4.2904312843,0.
H,0,-1.7248430438,-5.2905769429,0.
H,0,-3.3099473356,-4.2832988636,0.
O,0,1.9826278561,4.5555092219,0.
O,0,0.4971437781,0.5163517725,0.
O,0,-1.5569866697,-3.2762824654,0.
Recover connectivity data from disk.
Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.563770	3.428442	0.000000
2	1	0	2.228228	2.542248	0.000000
3	1	0	0.481755	3.191396	0.000000
4	6	0	-0.082090	-0.538679	0.000000
5	1	0	0.449731	-1.508691	0.000000
6	1	0	-1.186053	-0.611694	0.000000
7	6	0	-2.201872	-4.290431	0.000000
8	1	0	-1.724843	-5.290577	0.000000
9	1	0	-3.309947	-4.283299	0.000000
10	8	0	1.982628	4.555509	0.000000
11	8	0	0.497144	0.516352	0.000000
12	8	0	-1.556987	-3.276282	0.000000

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	H	1.107630	0.000000			
3	H	1.107676	1.863212	0.000000		
4	C	4.294986	3.850933	3.772450	0.000000	
5	H	5.061261	4.424156	4.700195	1.106235	0.000000
6	H	4.887149	4.648082	4.152719	1.106375	1.865581
7	C	8.588426	8.143175	7.948559	4.309190	3.843056
8	H	9.318598	8.773820	8.764299	5.027839	4.362503
9	H	9.122723	8.789737	8.381412	4.943808	4.672647
10	O	1.202382	2.028186	2.028158	5.496710	6.254941
11	O	3.101284	2.664753	2.675088	1.203579	2.025597
12	O	7.395435	6.941408	6.781396	3.109629	2.674191

		6	7	8	9	10
6	H	0.000000				
7	C	3.816411	0.000000			
8	H	4.709803	1.108083	0.000000		
9	H	4.241652	1.108099	1.878075	0.000000	
10	O	6.061397	9.785740	10.520967	10.302227	0.000000
11	O	2.026238	5.512699	6.217527	6.126221	4.303656
12	O	2.690283	1.201821	2.021276	2.021621	8.594523

```
            11        12
  11  O    0.000000
  12  O    4.313181   0.000000
                   Interatomic angles:
    H2-C1-H3=114.5051       H5-C4-H6=114.9504       H8-C7-H9=115.868
    H2-C1-O10=122.751       H3-C1-O10=122.7439      H2-H3-O10= 62.6567
    C1-H2-O11=102.6247      C1-H3-O11=102.0275      H3-H2-O11= 69.8765
    H2-O11-C4=168.2545      H3-O11-C4=150.9027      H2-O11-H5=140.8281
    H3-O11-H5=178.3292      H5-C4-O11=122.498       H2-O11-H6=164.3424
    H3-O11-H6=123.4996      H6-C4-O11=122.5516      H6-H5-O11= 62.6027
   O10-H2-O11=132.5316     O10-H3-O11=131.9375      C4-H5-O12=102.6405
    C4-H6-O12=101.7091      H6-H5-O12= 70.1134      H5-O12-C7=163.8266
    H6-O12-C7=155.4733      H5-O12-H8=136.1384      H6-O12-H8=176.8385
    H8-C7-O12=122.049       H5-O12-H9=168.5011      H6-O12-H9=127.801
    H9-C7-O12=122.083       H9-H8-O12= 62.3291     O11-H5-O12=132.716
   O11-H6-O12=131.7543
Stoichiometry    C3H6O3
Framework group  CS[SG(C3H6O3)]
Deg. of freedom   21
Full point group                 CS      NOp   2
Largest Abelian subgroup         CS      NOp   2
Largest concise Abelian subgroup C1      NOp   1
                    Standard orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type             X           Y           Z
---------------------------------------------------------------------
    1          6           0       -1.029422   -3.624897    0.000000
    2          1           0       -1.819803   -2.848919    0.000000
    3          1           0        0.004532   -3.227549    0.000000
    4          6           0        0.000000    0.544898    0.000000
    5          1           0       -0.671885    1.423719    0.000000
    6          1           0        1.080364    0.783394    0.000000
    7          6           0        1.530381    4.573180    0.000000
    8          1           0        0.908123    5.490046    0.000000
    9          1           0        2.626885    4.733062    0.000000
   10          8           0       -1.273705   -4.802203    0.000000
   11          8           0       -0.413681   -0.585354    0.000000
   12          8           0        1.045639    3.473453    0.000000
---------------------------------------------------------------------
Rotational constants (GHZ):     70.1259093      0.4410420      0.4382855
Isotopes: C-12,H-1,H-1,C-12,H-1,H-1,C-12,H-1,H-1,O-16,O-16,O-16
Standard basis: CBSB3 (5D, 7F)
There are   186 symmetry adapted basis functions of A'  symmetry.
There are    78 symmetry adapted basis functions of A"  symmetry.
Crude estimate of integral set expansion from redundant integrals=1.000.
Integral buffers will be    262144 words long.
Raffenetti 1 integral format.
Two-electron integral symmetry is turned on.
  264 basis functions      384 primitive gaussians
   24 alpha electrons       24 beta electrons
      nuclear repulsion energy       175.9786698479 Hartrees.
One-electron integrals computed using PRISM.
NBasis=   264 RedAO= T  NBF=   186    78
NBsUse=   264 1.00D-04 NBFU=   186    78
Initial guess read from the checkpoint file:
C:\Users\hp\Desktop\3_cbsqb3.chk
Initial guess orbital symmetries:
      Occupied  (A') (A') (A') (A') (A') (A') (A') (A') (A')
                (A') (A') (A') (A') (A') (A') (A') (A") (A")
                (A") (A') (A') (A')
      Virtual   (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
                (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
                (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
                (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
                (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
                (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
                (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
                (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
                (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
                (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
                (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
                (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
                (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
```

(A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
(A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
(A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
(A') (A') (A') (A') (A') (A") (A") (A") (A") (A")
(A") (A") (A") (A") (A") (A") (A") (A") (A") (A")
(A") (A") (A") (A") (A") (A") (A") (A") (A") (A")
(A") (A") (A") (A") (A") (A") (A") (A") (A") (A")
(A") (A") (A") (A") (A") (A") (A") (A") (A") (A")
(A") (A") (A") (A") (A") (A") (A") (A") (A") (A")
(A") (A") (A") (A") (A") (A") (A") (A") (A") (A")
Requested convergence on RMS density matrix=1.00D-08 within 64 cycles.
Requested convergence on MAX density matrix=1.00D-06.
SCF Done: E(RHF) = -341.736610121 A.U. after 11 cycles
Convg = 0.2116D-08 -V/T = 2.0015
S**2 = 0.0000
Range of M.O.s used for correlation: 7 264
NBasis= 264 NAE= 24 NBE= 24 NFC= 6 NFV= 0
NROrb= 258 NOA= 18 NOB= 18 NVA= 240 NVB= 240

**** Warning!!: The largest alpha MO coefficient is 0.14954698D+02

Semi-Direct transformation.
ModeAB= 4 MOrb= 4 LenV= 5027064
LASXX= 23723181 LTotXX= 23723181 LenRXX= 48098862
LTotAB= 24375681 MaxLAS= 144349452 LenRXY= 0
NonZer= 71822043 LenScr= 112734720 LnRSAI= 32077656
LnScr1= 53078016 LExtra= 4310690 Total= 250299944
MaxDsk= 262144000 SrtSym= T ITran= 3
JobTyp=0 Pass 1: I= 1 to 2.
JobTyp=0 Pass 2: I= 3 to 6.
JobTyp=0 Pass 3: I= 7 to 10.
JobTyp=0 Pass 4: I= 11 to 14.
JobTyp=0 Pass 5: I= 15 to 18.
Spin components of T(2) and E(2):
alpha-alpha T2 = 0.4050759265D-01 E2= -0.1418130747D+00
alpha-beta T2 = 0.2477951672D+00 E2= -0.8881458363D+00
beta-beta T2 = 0.4050759265D-01 E2= -0.1418130747D+00
ANorm= 0.1152740366D+01
E2= -0.1171771986D+01 EUMP2= -0.34290838210698D+03

Complete Basis Set (CBS) Extrapolation:
M. R. Nyden and G. A. Petersson, JCP 75, 1843 (1981)
G. A. Petersson and M. A. Al-Laham, JCP 94, 6081 (1991)
G. A. Petersson, T. Tensfeldt, and J. A. Montgomery, JCP 94, 6091 (1991)
J. A. Montgomery, J. W. Ochterski, and G. A. Petersson, JCP 101, 5900 (1994)

Minimum Number of PNO for Extrapolation = 10
Absolute Overlaps: IRadAn = 99302
LocTrn: ILocal=3 LocCor=F DoCore=F.
LocMO: Using population method
Initial Trace= 0.18000000D+02 Initial TraceA= 0.77735193D+01
RMSG= 0.21134959D-08
E2(CBS)= -1.289299 CBS-Int= 0.037948 OIii= 10.014759

****

Population analysis using the SCF density.

****

Orbital Symmetries:
Occupied (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
(A') (A') (A') (A') (A') (A') (A') (A') (A") (A")
(A") (A') (A') (A')
Virtual (A') (A') (A') (A") (A') (A') (A") (A") (A') (A')
(A') (A') (A") (A') (A') (A") (A") (A') (A') (A')
(A') (A') (A') (A') (A') (A") (A') (A') (A') (A")
(A') (A') (A") (A') (A') (A') (A') (A') (A') (A')
(A') (A') (A') (A') (A') (A') (A') (A") (A") (A')
(A") (A") (A") (A') (A") (A') (A') (A') (A') (A')
(A") (A") (A') (A') (A") (A') (A') (A') (A') (A')
(A') (A') (A") (A") (A") (A') (A") (A") (A") (A')
(A') (A') (A') (A') (A") (A") (A') (A") (A') (A')

(A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
(A') (A') (A') (A') (A") (A') (A") (A") (A') (A')
(A') (A") (A") (A") (A') (A') (A') (A') (A') (A')
(A') (A') (A') (A') (A') (A') (A") (A") (A") (A")
(A") (A") (A") (A") (A") (A') (A') (A') (A') (A')
(A') (A') (A') (A') (A') (A') (A') (A") (A") (A")
(A") (A') (A") (A') (A") (A') (A') (A") (A') (A")
(A') (A") (A') (A') (A') (A') (A') (A') (A') (A")
(A') (A") (A") (A") (A') (A") (A") (A') (A') (A')
(A') (A') (A') (A') (A') (A') (A') (A") (A') (A")
(A') (A") (A") (A") (A") (A') (A') (A') (A') (A")
(A') (A") (A') (A') (A') (A") (A') (A') (A') (A')
(A") (A") (A") (A') (A') (A') (A") (A") (A') (A")
(A') (A') (A') (A') (A') (A") (A") (A") (A') (A')
(A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
The electronic state is 1-A'.
Alpha occ. eigenvalues -- -20.60108 -20.57381 -20.55049 -11.36549 -11.33590
Alpha occ. eigenvalues -- -11.31172 -1.43429 -1.40659 -1.38259 -0.89234
Alpha occ. eigenvalues -- -0.86332 -0.83747 -0.71683 -0.68762 -0.68296
Alpha occ. eigenvalues -- -0.66323 -0.65277 -0.62390 -0.56506 -0.53861
Alpha occ. eigenvalues -- -0.51383 -0.46727 -0.43870 -0.41252
Alpha virt. eigenvalues -- 0.02855 0.04781 0.05431 0.05736 0.07081
Alpha virt. eigenvalues -- 0.07675 0.07802 0.09708 0.10266 0.11258
Alpha virt. eigenvalues -- 0.14270 0.14678 0.15164 0.16020 0.16241
Alpha virt. eigenvalues -- 0.17648 0.18679 0.19055 0.19749 0.20591
Alpha virt. eigenvalues -- 0.21158 0.23036 0.25520 0.27714 0.29804
Alpha virt. eigenvalues -- 0.30819 0.31810 0.32552 0.33628 0.34936
Alpha virt. eigenvalues -- 0.37052 0.38078 0.38249 0.40561 0.41561
Alpha virt. eigenvalues -- 0.43195 0.44822 0.46637 0.48973 0.50210
Alpha virt. eigenvalues -- 0.58981 0.63051 0.63975 0.64978 0.65225
Alpha virt. eigenvalues -- 0.65814 0.66984 0.67201 0.68886 0.69299
Alpha virt. eigenvalues -- 0.70181 0.71480 0.72362 0.72943 0.73899
Alpha virt. eigenvalues -- 0.74850 0.78795 0.79365 0.82990 0.86753
Alpha virt. eigenvalues -- 0.91338 0.96072 0.98082 0.99001 0.99306
Alpha virt. eigenvalues -- 1.03671 1.04007 1.06337 1.08369 1.09664
Alpha virt. eigenvalues -- 1.11065 1.14617 1.14801 1.15658 1.17450
Alpha virt. eigenvalues -- 1.18939 1.19356 1.19571 1.21508 1.23373
Alpha virt. eigenvalues -- 1.24752 1.27912 1.28604 1.31503 1.32064
Alpha virt. eigenvalues -- 1.36004 1.36052 1.37860 1.40545 1.43440
Alpha virt. eigenvalues -- 1.44475 1.47369 1.49362 1.61420 1.62080
Alpha virt. eigenvalues -- 1.63488 1.66026 1.66982 1.70037 1.70681
Alpha virt. eigenvalues -- 1.72158 1.73013 1.84042 1.88143 1.92609
Alpha virt. eigenvalues -- 1.92840 1.95154 1.97765 2.11828 2.14367
Alpha virt. eigenvalues -- 2.18352 2.18738 2.22255 2.25175 2.46879
Alpha virt. eigenvalues -- 2.49502 2.50185 2.69759 2.75751 2.81012
Alpha virt. eigenvalues -- 2.82893 2.84512 2.85531 2.87034 2.89597
Alpha virt. eigenvalues -- 2.91904 3.01648 3.04778 3.06884 3.15829
Alpha virt. eigenvalues -- 3.18269 3.18777 3.21031 3.21176 3.22966
Alpha virt. eigenvalues -- 3.30131 3.32588 3.34065 3.35162 3.36320
Alpha virt. eigenvalues -- 3.36970 3.38672 3.40771 3.41371 3.43386
Alpha virt. eigenvalues -- 3.46996 3.47699 3.49412 3.53195 3.55941
Alpha virt. eigenvalues -- 3.56108 3.56831 3.58901 3.59942 3.61281
Alpha virt. eigenvalues -- 3.62515 3.84607 3.85962 3.88804 3.88998
Alpha virt. eigenvalues -- 3.90194 3.91610 4.06060 4.10623 4.11317
Alpha virt. eigenvalues -- 4.14014 4.17597 4.20103 4.34063 4.38921
Alpha virt. eigenvalues -- 4.41063 4.42024 4.42506 4.43760 4.44148
Alpha virt. eigenvalues -- 4.46181 4.48407 4.53134 4.56697 4.57918
Alpha virt. eigenvalues -- 4.86562 4.90917 4.94353 5.32639 5.34102
Alpha virt. eigenvalues -- 5.36624 5.45139 5.47652 5.48009 5.50209
Alpha virt. eigenvalues -- 5.50435 5.52675 5.56482 5.60005 5.61903
Alpha virt. eigenvalues -- 5.68004 5.71784 5.73863 5.84259 5.85449
Alpha virt. eigenvalues -- 5.87353 5.88127 5.88659 5.89499 5.90337
Alpha virt. eigenvalues -- 5.90919 5.91471 6.29015 6.32584 6.35226
Alpha virt. eigenvalues -- 6.70093 6.72287 6.75239 6.99385 7.02608
Alpha virt. eigenvalues -- 7.05742 7.32461 7.35078 7.36392 7.37518
Alpha virt. eigenvalues -- 7.39525 7.41193 7.52690 7.58442 7.63553
Alpha virt. eigenvalues -- 7.67086 7.70230 7.72773 7.85393 7.88306
Alpha virt. eigenvalues -- 7.90620 8.12788 8.19439 8.19547 25.68094
Alpha virt. eigenvalues -- 25.70870 25.73216 51.79802 51.82937 51.85133
Condensed to atoms (all electrons):

		1	2	3	4	5	6
1	C	4.539535	0.424213	0.416472	-0.011092	0.000276	0.000486
2	H	0.424213	0.629686	-0.079006	0.001220	0.001465	-0.001602
3	H	0.416472	-0.079006	0.633984	0.001031	-0.001387	0.001645

```
 4  C   -0.011092   0.001220   0.001031   4.700215   0.434479   0.426209
 5  H    0.000276   0.001465  -0.001387   0.434479   0.583565  -0.060450
 6  H    0.000486  -0.001602   0.001645   0.426209  -0.060450   0.589076
 7  C   -0.000013  -0.000016  -0.000003  -0.013167   0.001505   0.000623
 8  H    0.000000  -0.000001   0.000004  -0.000035   0.002393  -0.001970
 9  H    0.000000   0.000003  -0.000001   0.000281  -0.002146   0.002627
10  O    0.459413  -0.059187  -0.064207   0.001133   0.000037   0.000004
11  O    0.011959  -0.005389  -0.011971   0.280881  -0.063823  -0.062078
12  O    0.000012   0.000025   0.000036   0.025541  -0.009034  -0.010756
             7          8          9         10         11         12
 1  C   -0.000013   0.000000   0.000000   0.459413   0.011959   0.000012
 2  H   -0.000016  -0.000001   0.000003  -0.059187  -0.005389   0.000025
 3  H   -0.000003   0.000004  -0.000001  -0.064207  -0.011971   0.000036
 4  C   -0.013167  -0.000035   0.000281   0.001133   0.280881   0.025541
 5  H    0.001505   0.002393  -0.002146   0.000037  -0.063823  -0.009034
 6  H    0.000623  -0.001970   0.002627   0.000004  -0.062078  -0.010756
 7  C    4.701875   0.434062   0.430664   0.000000   0.000525   0.234272
 8  H    0.434062   0.611602  -0.068742   0.000000  -0.000022  -0.064552
 9  H    0.430664  -0.068742   0.613213   0.000000  -0.000024  -0.062553
10  O    0.000000   0.000000   0.000000   8.037153  -0.001577   0.000000
11  O    0.000525  -0.000022  -0.000024  -0.001577   8.240919  -0.001089
12  O    0.234272  -0.064552  -0.062553   0.000000  -0.001089   8.243967
Total atomic charges:
             1
 1  C    0.158738
 2  H    0.088588
 3  H    0.103403
 4  C    0.153304
 5  H    0.113120
 6  H    0.116187
 7  C    0.209673
 8  H    0.087262
 9  H    0.086676
10  O   -0.372769
11  O   -0.388310
12  O   -0.355870
Sum of Mulliken charges=   0.00000
Atomic charges with hydrogens summed into heavy atoms:
             1
 1  C    0.350729
 2  H    0.000000
 3  H    0.000000
 4  C    0.382610
 5  H    0.000000
 6  H    0.000000
 7  C    0.383611
 8  H    0.000000
 9  H    0.000000
10  O   -0.372769
11  O   -0.388310
12  O   -0.355870
Sum of Mulliken charges=   0.00000
Electronic spatial extent (au):  <R**2>=  2292.1867
Charge=     0.0000 electrons
Dipole moment (Debye):
   X=     3.0289    Y=     9.1517    Z=     0.0000  Tot=     9.6399
Quadrupole moment (Debye-Ang):
  XX=   -33.1235   YY=   -38.0060   ZZ=   -35.2455
  XY=     1.6364   XZ=     0.0000   YZ=     0.0000
Octapole moment (Debye-Ang**2):
 XXX=    12.0762  YYY=   305.6495  ZZZ=     0.0000  XYY=    89.2250
 XXY=    30.6797  XXZ=     0.0000  XZZ=    -0.1813  YZZ=    -0.4630
 YYZ=     0.0000  XYZ=     0.0000
Hexadecapole moment (Debye-Ang**3):
XXXX=  -261.6445 YYYY= -2656.4800 ZZZZ=   -31.4570 XXXY=  -342.1314
XXXZ=     0.0000 YYYX=  -348.9017 YYYZ=     0.0000 ZZZX=     0.0000
ZZZY=     0.0000 XXYY=  -430.5349 XXZZ=   -52.6349 YYZZ=  -424.4982
XXYZ=     0.0000 YYXZ=     0.0000 ZZXY=  -122.5134
N-N= 1.759786698479D+02 E-N=-1.157630702291D+03  KE= 3.412369553890D+02
Symmetry A'   KE= 3.307075964043D+02
Symmetry A"   KE= 1.052935898468D+01
1|1|UNPC-UNK|SP|RMP2-FC|CBSB3|C3H6O3|PCUSER|11-Oct-2015|0||#N GEOM=ALL
CHECK GUESS=TCHECK MP2/CBSB3 CBSEXTRAP=(NMIN=10,MINPOP)||Title Card Re
quired||0,1|C,1.5637698791,3.4284420444,0.|H,2.2282278702,2.5422482383
```

,0.|H,0.481755476,3.1913956349,0.|C,-0.0820898157,-0.5386793693,0.|H,0
.4497309692,-1.5086906652,0.|H,-1.1860533013,-0.6116939792,0.|C,-2.201
8717885,-4.2904312843,0.|H,-1.7248430438,-5.2905769429,0.|H,-3.3099473
356,-4.2832988636,0.|O,1.9826278561,4.5555092219,0.|O,0.4971437781,0.5
163517725,0.|O,-1.5569866697,-3.2762824654,0.||Version=x86-Win32-G98Re
vA.11.4|State=1-A'|HF=-341.7366101|MP2=-342.9083821|E2(CBS)=-1.2892994
|CBS-Int=-1.2513514|OIii=10.014759|RMSD=2.116e-009|PG=CS [SG(C3H6O3)]|
|@

IN SO FAR AS QUANTUM MECHANICS IS CORRECT, CHEMICAL
QUESTIONS ARE PROBLEMS IN APPLIED MATHEMATICS.

-- EYRING, WALTER, & KIMBALL, 1944
1 IMAGINARY FREQUENCIES IGNORED.

Complete Basis Set (CBS) Extrapolation:
M. R. Nyden and G. A. Petersson, JCP 75, 1843 (1981)
G. A. Petersson and M. A. Al-Laham, JCP 94, 6081 (1991)
G. A. Petersson, T. Tensfeldt, and J. A. Montgomery, JCP 94, 6091 (1991)
J. A. Montgomery, J. W. Ochterski, and G. A. Petersson, JCP 101, 5900 (1994)

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.080546 E(Thermal)= 0.092463
E(SCF)= -341.736610 DE(MP2)= -1.171772
DE(CBS)= -0.117527 DE(MP34)= -0.044733
DE(CCSD)= -0.029413 DE(Int)= 0.037948
DE(Empirical)= -0.057985
CBS-QB3 (0 K)= -343.039547 CBS-QB3 Energy= -343.027630
CBS-QB3 Enthalpy= -343.026686 CBS-QB3 Free Energy= -343.085563
1|1|UNPC-UNK|Mixed|CBS-QB3|CBS-QB3|C3H6O3|PCUSER|11-Oct-2015|0||# OPT
FREQ CBS-QB3 6-311++G(D,P) GEOM=CONNECTIVITY||Title Card Required||0,1
|C,1.5637698791,3.4284420444,0.|H,2.2282278702,2.5422482383,0.|H,0.481
755476,3.1913956349,0.|C,-0.0820898157,-0.5386793693,0.|H,0.4497309692
,-1.5086906652,0.|H,-1.1860533013,-0.6116939792,0.|C,-2.2018717885,-4.
2904312843,0.|H,-1.7248430438,-5.2905769429,0.|H,-3.3099473356,-4.2832
988636,0.|O,1.9826278561,4.5555092219,0.|O,0.4971437781,0.5163517725,0
.|O,-1.5569866697,-3.2762824654,0.||Version=x86-Win32-G98RevA.11.4|Sta
te=1-A'|HF/CbsB3=-341.7366101|E2(CBS)/CbsB3=-1.2892994|CBS-Int/CbsB3=0
.037948|OIii/CbsB3=10.014759|MP2/CbsB4=-342.6106131|MP4(SDQ)/CbsB4=-34
2.6553462|MP4(SDQ)/6-31+G(d')=-342.6047345|QCISD(T)/6-31+G(d')=-342.63
41479|CBSQB3=-343.039547|FreqCoord=2.9550965807,6.4788160317,0.,4.2107
401148,4.8041525653,0.,0.9103858431,6.030863271,0.,-0.1551272581,-1.01
79564036,0.,0.8498683003,-2.8510119588,0.,-2.2413157474,-1.1559340096,
0.,-4.1609343422,-8.1077395001,0.,-3.2594807262,-9.9977407435,0.,-6.25
48935009,-8.0942611794,0.,3.7466233853,8.6086641679,0.,0.9394655175,0.
9757633638,0.,-2.9422781735,-6.1912761207,0.|PG=CS [SG(C3H6O3)]|NImag=
1||0.63020900,0.13390753,0.94183930,0.00000003,0.00000006,0.17788203,-
0.16485221,0.10116149,0.,0.15342753,0.11013502,-0.16750009,-0.00000002
,-0.11581240,0.21480808,-0.00000004,-0.00000011,-0.05997609,0.,0.00000
004,0.02041973,-0.27018447,-0.01197982,-0.00000003,-0.01691165,-0.0027
9546,0.00000004,0.29398597,-0.02119569,-0.06168615,-0.00000001,0.02146
145,0.00485503,0.00000007,0.04737485,0.07386069,-0.00000007,-0.0000001
1,-0.05994706,-0.00000002,0.00000002,0.02030416,0.00000005,-0.00000002
,0.02040171,-0.00103152,-0.00122698,-0.00000003,-0.00026243,0.00002503
,-0.00000015,0.00052692,-0.00084357,0.00000026,0.68043261,-0.00137447,
-0.00311707,-0.00000006,-0.00090846,-0.00040886,0.00000022,0.00054972,
-0.00067422,-0.00000004,0.17028429,0.89833845,-0.00000019,-0.00000041,
0.00003692,-0.00000002,0.00000011,0.00002297,0.00000017,0.00000011,0.0
0004217,0.00000010,0.00000042,0.17806789,-0.00000689,-0.00017528,0.,-0
.00001263,-0.00003621,-0.00000004,-0.00002837,0.00011753,0.00000002,-0
.13642045,0.09917842,-0.00000005,0.12312839,0.00066831,0.00031296,0.,0
.00014010,0.00011645,0.,-0.00031847,0.00033329,-0.00000002,0.10720940,
-0.20070085,-0.00000004,-0.10407130,0.24878270,-0.00000023,-0.00000044
,-0.00000014,-0.00000005,0.00000010,-0.00002742,0.00000020,0.00000002,
0.00010775,0.00000052,0.00000018,-0.06012199,0.00000002,-0.00000006,0.
02062263,-0.00014085,0.00058346,0.,0.00030452,0.00000384,0.00000017,-0
.00004799,0.00019304,-0.00000017,-0.27497054,0.01859068,0.00000010,-0.
01309147,-0.00049573,-0.00000024,0.30631032,-0.00033175,0.00025942,0.,
0.00029842,0.00008393,-0.00000007,0.00002467,0.00001839,0.00000006,0.0
1051023,-0.06153646,-0.00000006,0.02399242,0.00198036,0.00000007,0.012
94713,0.06491004,0.00000043,0.00000090,-0.00000485,0.00000007,-0.00000
023,0.00008921,-0.00000039,-0.00000016,-0.00004194,-0.00000055,-0.0000
0069,-0.06014569,0.00000005,0.00000010,0.02033567,0.00000006,0.0000000

3,0.02059682,-0.00003252,-0.00036744,-0.00000005,-0.00011966,0.0000014
3,0.00000039,0.00004071,-0.00007795,-0.00000023,-0.00121903,-0.0014315
4,0.00000049,-0.00025316,0.00004056,-0.00000012,0.00031443,-0.00086951
,-0.00000053,0.69680085,-0.00033346,-0.00060962,-0.00000007,-0.0001379
5,-0.00000774,-0.00000026,0.00016879,-0.00010353,0.00000054,-0.0014468
4,-0.00273486,0.00000030,-0.00099090,-0.00026653,0.00000113,0.00033940
,-0.00060471,-0.00000132,0.18689524,0.87240105,0.00000008,0.00000016,0
.00000569,0.00000001,-0.00000004,0.00000395,-0.00000007,-0.00000004,0.
00000395,-0.00000006,-0.00000015,0.00003897,0.00000001,0.00000002,0.00
003235,-0.00000002,0.00000002,0.00003997,-0.00000016,-0.00000017,0.175
65931,-0.00002710,-0.00002372,0.00000001,0.00000257,0.00000379,-0.0000
0025,0.00001286,0.00000604,0.00000023,0.00007331,-0.00009218,-0.000000
17,-0.00001466,-0.00003042,0.00000031,-0.00003126,0.00015236,-0.000000
03,-0.12521620,0.09456329,0.00000004,0.11188097,0.00009829,0.00014575,
0.,0.00002683,-0.00000229,0.00000046,-0.00005187,0.00001505,-0.0000004
7,0.00072005,0.00023932,0.00000024,0.00018216,0.00009707,-0.00000069,-
0.00026657,0.00038105,0.00000025,0.09822241,-0.20735685,-0.00000004,-0
.09386389,0.25611018,-0.00000044,-0.00000094,0.00000192,-0.00000006,0.
00000025,0.00000131,0.00000040,0.00000022,0.00000141,0.00000038,0.0000
0085,0.00000515,-0.00000008,-0.00000010,-0.00003198,0.00000010,-0.0000
0009,0.00009936,0.00000086,0.00000101,-0.05894580,-0.00000019,0.000000
18,0.01989587,0.00000437,0.00010635,0.,0.00003622,-0.00000080,0.,-0.00
001092,0.00002236,0.,-0.00007891,0.00066573,-0.00000002,0.00033255,-0.
00003020,0.,-0.00001330,0.00019762,0.00000003,-0.26644244,0.03191592,0
.,-0.01057706,0.00142693,-0.00000004,0.30212363,0.00001209,0.00004267,
0.,0.00001438,0.00000001,0.00000002,-0.00001038,0.00000908,-0.00000005
,-0.00023314,0.00033812,-0.00000003,0.00031782,0.00004389,-0.00000010,
0.00000026,0.00003191,0.00000012,0.02819651,-0.06601948,0.00000002,0.0
2416229,0.00143894,-0.00000009,-0.00457099,0.06573458,0.00000026,0.000
00057,0.00000181,0.00000003,-0.00000015,0.00000130,-0.00000024,-0.0000
0014,0.00000122,-0.00000020,-0.00000053,-0.00000293,0.00000005,0.00000
006,0.00009469,-0.00000008,0.00000007,-0.00003604,-0.00000056,-0.00000
056,-0.05897883,0.00000015,-0.00000017,0.01975974,0.00000002,0.0000000
5,0.01989308,-0.19223320,-0.22348484,0.,0.02735495,0.00942683,-0.00000
001,-0.00731325,-0.04761128,0.00000003,0.00063552,0.00109462,0.0000000
3,0.00002762,-0.00036156,0.00000008,-0.00005989,0.00004570,-0.00000011
,0.00008082,0.00023860,-0.00000002,0.00001062,-0.00005804,0.00000009,-
0.00002092,-0.00001178,-0.00000005,0.17152214,-0.22335424,-0.71075757,
-0.00000003,-0.00754264,-0.05156008,0.00000002,-0.03093363,-0.01693823
,0.00000010,0.00140915,0.00273552,0.00000020,0.00007758,-0.00050349,0.
00000030,-0.00052143,-0.00021294,-0.00000050,0.00033680,0.00056270,-0.
00000009,0.00001511,-0.00012601,0.00000049,-0.00009637,-0.00003832,-0.
00000029,0.26269854,0.78084606,0.00000008,0.00000017,-0.05845036,0.000
00001,-0.00000004,0.01956210,-0.00000007,-0.00000003,0.01957505,-0.000
00009,-0.00000014,-0.00004285,0.00000001,0.00000002,-0.00000707,0.,0.,
-0.00001259,-0.00000012,-0.00000022,-0.00000870,0.,0.00000002,-0.00000
301,0.,0.00000002,-0.00000284,-0.00000002,-0.00000009,0.01934275,-0.00
177593,0.00110827,0.00000003,0.00090713,-0.00095327,0.00000003,-0.0000
0985,0.00047298,-0.00000013,-0.26637970,-0.28790147,-0.00000016,0.0255
3402,-0.00167699,-0.00000033,-0.01842104,-0.04743945,0.00000047,0.0008
8137,0.00132210,0.00000007,-0.00002588,-0.00044560,-0.00000042,-0.0001
5053,-0.00002473,0.00000024,0.00009790,-0.00172705,0.00000008,0.259756
82,0.00145617,0.00044965,0.00000005,0.00113484,-0.00040924,-0.00000016
,-0.00187236,0.00017052,0.,-0.28782778,-0.63279148,-0.00000034,-0.0195
4393,-0.04968866,-0.00000021,-0.02976908,-0.00573234,0.00000061,0.0015
2493,0.00244122,0.00000013,-0.00000896,-0.00047338,-0.00000072,-0.0005
7589,-0.00027173,0.00000044,-0.00172704,-0.00340395,0.00000012,0.33928
963,0.69265820,0.,0.,0.00046328,0.,0.,-0.00039070,0.,0.00000002,-0.000
43781,-0.00000008,0.00000005,-0.05831432,-0.00000001,0.,0.01938985,0.0
0000007,-0.00000003,0.01949848,0.00000013,-0.00000015,-0.00004059,-0.0
0000009,0.00000018,-0.00000901,0.,0.00000001,-0.00001152,0.,-0.0000000
1,0.00002764,0.00000003,-0.00000004,0.01980215,0.00007131,0.00039100,0
.00000004,0.00012566,0.00000220,-0.00000015,-0.00005997,0.00008023,0.0
0000002,-0.00130579,0.00134465,-0.00000029,0.00080506,-0.00107369,-0.0
0000014,-0.00015294,0.00047216,0.00000050,-0.30483518,-0.31253419,0.00
000011,0.02391180,-0.00599069,-0.00000060,-0.02520270,-0.04785234,0.00
000037,-0.00010233,-0.00036182,0.00000010,-0.00041432,-0.00208053,-0.0
0000004,0.30715939,0.00031222,0.00062075,0.00000007,0.00016393,0.00002
479,-0.00000023,-0.00015604,0.00014008,0.,0.00142015,0.00031238,-0.000
00050,0.00095170,-0.00050720,-0.00000030,-0.00160500,0.00042135,0.0000
0090,-0.31247145,-0.59770164,0.00000019,-0.02488371,-0.05046883,-0.000
00105,-0.02906065,-0.00130968,0.00000065,-0.00024975,-0.00060371,0.000
00017,-0.00202442,-0.00294880,-0.00000005,0.36760301,0.65202052,0.0000
0008,0.00000016,-0.00001315,0.00000001,-0.00000004,-0.00001052,-0.0000

0007,-0.00000003,-0.00001060,-0.00000010,-0.00000013,0.00041372,0.,0.0
0000002,-0.00039435,0.00000001,0.,-0.00041840,-0.00000010,-0.00000024,
-0.05781028,0.,0.00000005,0.01922505,0.,0.00000002,0.01928033,-0.00000
002,-0.00000009,0.00001988,0.00000009,0.00000011,0.00002254,0.00000009
,0.00000016,0.01969577||-0.00000749,0.00001770,0.,-0.00004535,-0.00003
297,0.,-0.00000049,0.00000023,0.,-0.00003821,0.00005961,0.,-0.00000696
,0.00000572,0.,-0.00000113,0.00004057,0.,0.00000404,0.00006819,0.,0.00
000718,-0.00000866,0.,-0.00001143,0.00000282,0.,0.00000135,-0.00002278
,0.,0.00009875,0.00000929,0.,-0.00000027,-0.00013973,0.|||@
Job cpu time: * days * hours * minutes   * seconds.
File lengths (MBytes): RWF= 1993 Int=   0 D2E=   0 Chk=   6 Scr=   1
Normal termination of Gaussian 98.