

TABLE 1S: Structure,^a rotational constants, dipole moment and energy differences of *Syn* 1, *Skew* 1 and *Skew* 3 of 1-ethenylcyclopropan-1-ol as calculated at the B3LYP/6-31G* level of theory

Conformer:	<i>Syn</i> 1	<i>Skew</i> 1	<i>Skew</i> 3
Bond length/pm			
O1-H1	97.2	96.4	96.3
C1-O1	140.6	140.9	140.9
C1-C2	148.4	148.0	148.1
C2-C3	133.5	133.5	133.5
C2-H2	109.0	108.5	108.6
C3-H3	108.6	108.0	108.0
C3-H4	108.6	108.1	108.0
C1-C4	150.9	149.6	151.0
C1-C5	152.2	150.1	148.9
C4-H5	108.6	107.9	107.9
C4-H6	108.6	107.9	108.0
C5-H7	108.6	107.9	107.8
C5-H8	108.7	107.9	107.8
Angle/°			
H1-O1-C1	106.9	106.5	107.1
O1-C1-C2	116.0	114.0	114.6
C1-C2-C3	124.6	125.6	126.3
C1-C2-H2	115.4	114.6	114.8
C2-C3-H3	121.5	120.9	120.8
C2-C3-H4	121.3	121.5	121.7
O1-C1-C4	113.6	112.9	116.4
O1-C1-C5	116.8	117.0	113.7
C1-C4-H5	118.2	117.6	117.6
C1-C4-H6	115.5	115.8	116.5
C1-C5-H7	116.1	115.8	115.2
C1-C5-H8	118.7	119.3	119.0

(Table 1 continued next page)

(Table 1 continued)

Dihedral angle ^b /°			
H1-O1-C1-C2	-65.5	-67.1	72.9
O1-C1-C2-C3	-4.3	132.1	135.3
O1-C1-C2-H2	174.9	-47.6	-45.7
C1-C2-C3-H3	179.1	179.0	178.0
C1-C2-C3-H4	-2.1	-0.8	-2.2
H1-O1-C1-C4	149.6	151.6	-72.7
H1-O1-C1-C5	83.0	83.9	-140.4
O1-C1-C4-H5	142.4	143.2	148.9
O1-C1-C4-H6	0.4	-1.3	3.3
O1-C1-C5-H7	-5.0	-4.7	0.2
O1-C1-C5-H8	-148.4	-150.6	-144.2
Rotational constants/MHz			
<i>A</i>	6412.6	5505.7	5507.0
<i>B</i>	2913.9	3180.7	3192.7
<i>C</i>	2401.6	2517.8	2506.3
Dipole moment ^c /10 ⁻³⁰ C m			
μ_a	0.22	3.34	0.97
μ_b	2.31	1.83	0.97
μ_c	4.10	2.94	5.13
μ_{tot}	4.68	4.80	5.30
Energy difference ^d /kJ mol ⁻¹			
	0.0 ^e	6.97	12.35

^aAtom numbering is given in Fig. 1. ^bMeasured from syn = 0°. ^c1 Debye = 3.33564 × 10³⁰ C m. ^dRelative to Syn 1. ^eTotal energy obtained in the B3LYP/6-31G* computations: -710202.93 kJ mol⁻¹.

Table 2S: Microwave Spectrum of the *Syn*1 conformer of 1-Ethenylcyclopropan-1-ol. (Parent species)

CALCULATION BY ASMIX.

D1 = DJ, D2 = DJK, D3 = DK, D4 = SDJ, D5 = SDJK, (KHZ)
 D6 = HJ, D7 = HJK, D8 = HKJ, D9 = HK,
 D10 = SHJ, D11 = SHJK, D12 = SHK, (HZ).

TOTAL NUMBER OF ACCEPTED TRANSITIONS: 324

FIXED CONSTANTS:

G- A = 0.000000
 G- B = 0.000000
 G- C = 0.000000
 MU -AB = 0.000000
 MU -BC = 0.000000
 D6 -LOWER = 0.00000000
 D7 -LOWER = 0.00000000
 D8 -LOWER = 0.00000000
 D9 -LOWER = 0.00000000
 D10 -LOWER = 0.00000000
 D11 -LOWER = 0.00000000
 D12 -LOWER = 0.00000000
 D6 -UPPER = 0.00000000
 D7 -UPPER = 0.00000000
 D8 -UPPER = 0.00000000
 D9 -UPPER = 0.00000000
 D10 -UPPER = 0.00000000
 D11 -UPPER = 0.00000000
 D12 -UPPER = 0.00000000

ACCURACY: ± 0.10 MHz

LABEL OF 0+ STATE: 0; LABEL OF 0- STATE: 1

VIB. ST.		TRANSITION		OBS. - OBS. FREQ. CALC.	
J' K' - 'K+'	J'' K'' - 'K+'				
0 0	3 1 3	4 0 4	18512.310	-0.127	
0 0	4 1 4	5 0 5	24055.210	-0.249	
0 0	5 0 5	6 1 6	31388.110	0.148	
0 0	5 1 5	6 0 6	29434.470	0.192	
0 0	6 1 6	7 0 7	34647.240	0.042	
0 0	6 2 5	7 1 6	32144.860	-0.098	
0 0	7 0 7	8 1 8	40454.430	0.170	
0 0	7 1 7	7 2 6	18836.730	0.132	
0 0	7 1 7	8 0 8	39725.040	-0.007	
0 0	8 1 8	8 2 7	21011.810	0.009	
0 0	8 1 8	9 0 9	44706.610	-0.082	
0 0	8 2 7	9 1 8	44654.390	-0.059	
0 0	9 0 9	9 1 8	20959.550	-0.007	
0 0	9 1 8	10 2 9	54829.370	0.012	
0 0	9 1 9	9 2 8	23388.760	0.154	
0 0	10 0 10	10 1 9	24285.820	-0.139	
0 0	10 1 9	10 2 8	16048.200	-0.192	
0 0	10 1 9	11 2 10	58938.930	0.029	
0 0	10 1 10	10 2 9	25927.680	0.193	
0 0	10 1 10	11 0 11	54505.480	-0.136	
0 0	10 2 9	10 3 8	23809.870	0.179	
0 0	10 2 9	11 1 10	56111.400	-0.082	
0 0	11 0 11	11 1 10	27533.470	0.117	
0 0	11 1 10	11 2 9	19147.110	0.028	
0 0	11 1 11	11 2 10	28589.690	0.188	
0 0	11 1 11	12 0 12	59362.780	-0.107	
0 0	11 2 10	11 3 9	25599.040	0.300	
0 0	12 0 12	12 1 11	30686.830	0.168	
0 0	12 1 11	12 2 10	22585.940	0.050	
0 0	12 1 12	12 2 11	31340.070	0.145	
0 0	12 2 10	12 3 9	15699.890	0.256	
0 0	12 2 11	12 3 10	27647.650	0.237	
0 0	13 0 13	13 1 12	33758.610	-0.034	
0 0	13 1 12	13 2 11	26176.170	0.101	
0 0	13 2 12	13 3 11	29924.340	0.222	

0	0	14	0	14	14	1	13	36770.410	0.281
0	0	14	1	13	14	2	12	29760.980	0.110
0	0	14	2	13	14	3	12	32390.850	0.213
0	0	14	3	12	14	4	11	30264.190	0.174
0	0	15	0	15	15	1	14	39740.120	0.019
0	0	15	1	14	15	2	13	33246.720	0.297
0	0	15	2	13	15	3	12	23472.090	-0.048
0	0	15	2	14	15	3	13	35006.970	0.230
0	0	15	3	12	15	4	11	18724.160	0.584
0	0	15	3	13	15	4	12	31940.090	0.262
0	0	16	1	15	16	2	14	36601.260	0.145
0	0	16	2	14	16	3	13	27105.040	-0.018
0	0	16	2	15	16	3	14	37734.590	0.252
0	0	16	3	13	16	4	12	19730.950	0.317
0	0	16	3	14	16	4	13	33892.860	0.251
0	0	16	4	12	16	5	11	24987.720	0.129
0	0	17	2	15	17	3	14	30938.450	0.019
0	0	17	2	16	17	3	15	40540.610	0.183
0	0	17	3	15	17	4	14	36094.390	0.216
0	0	18	2	16	18	3	15	34786.390	-0.234
0	0	18	3	15	18	4	14	24188.160	-0.063
0	0	18	3	16	18	4	15	38508.340	0.459
0	0	19	2	17	19	3	16	38527.080	0.137
0	0	19	4	15	19	5	14	22860.450	0.765
0	0	20	4	16	20	5	15	23654.750	0.329
0	0	21	4	17	21	5	16	25354.160	0.029
0	0	22	4	18	22	5	17	27936.520	-0.167
0	0	23	4	19	23	5	18	31290.010	-0.260
0	0	24	4	20	24	5	19	35219.270	-0.251
0	0	24	5	19	24	6	18	27516.360	0.342
0	0	25	4	21	25	5	20	39480.070	-0.267
0	0	25	4	21	25	5	20	39480.110	-0.227
0	0	25	5	20	25	6	19	29046.370	-0.115
0	0	26	5	21	26	6	20	31544.220	-0.314
0	0	27	5	22	27	6	21	34904.470	-0.283
0	0	28	5	23	28	6	22	38930.930	-0.379
0	0	28	5	23	28	6	22	38930.920	-0.389
0	0	28	6	22	28	7	21	31347.500	0.317
0	0	29	6	23	29	7	22	32673.050	-0.140
0	0	30	6	24	30	7	23	35047.440	-0.462
0	0	31	6	25	31	7	24	38375.130	-0.646
0	0	31	7	24	31	8	23	35188.140	0.352
0	0	32	7	25	32	8	24	35171.510	-0.510
0	0	33	7	26	33	8	25	36260.490	-0.514
0	0	34	7	27	34	8	26	38474.640	-0.704
0	0	36	8	28	36	9	27	39009.810	0.146
0	0	37	8	29	37	9	28	39831.260	-0.465
0	1	2	1	1	3	2	1	28950.280	0.335
0	1	2	1	2	3	2	2	30248.680	0.060
0	1	2	2	0	3	3	0	36865.180	0.070
0	1	2	2	1	3	3	1	36916.950	0.345
0	1	3	0	3	4	1	3	30121.900	-0.009
0	1	3	1	2	4	2	2	34026.060	-0.115
0	1	4	0	4	5	1	4	37015.590	0.000
0	1	4	1	3	5	2	3	39282.520	-0.080
0	1	7	2	5	8	1	7	35510.420	-0.257
0	1	8	2	6	9	1	8	39083.800	-0.035
0	1	9	4	6	9	5	4	35227.260	-0.068
0	1	10	3	8	10	4	6	29220.530	0.183
0	1	10	4	7	10	5	5	35130.580	0.217
0	1	11	4	8	11	5	6	35084.330	0.340
0	1	12	3	10	12	4	8	32081.920	-0.011
0	1	12	4	9	12	5	7	35153.430	0.398
0	1	13	3	11	13	4	9	34631.070	-0.013
0	1	13	4	10	13	5	8	35431.670	0.372
0	1	14	3	12	14	4	10	38091.510	-0.008
0	1	14	4	11	14	5	9	36045.010	0.309
0	1	15	4	12	15	5	10	37149.760	0.143
0	1	16	4	12	16	5	12	24657.240	0.110
0	1	16	4	13	16	5	11	38921.220	-0.208
0	1	17	5	12	17	6	12	37325.630	-0.507
0	1	18	5	13	18	6	13	35130.580	-0.645
0	1	19	4	15	19	5	15	15521.090	-0.419
0	1	23	5	18	23	6	18	18620.100	-0.452
0	1	24	5	19	24	6	19	15176.580	-0.038
0	1	25	5	20	25	6	20	12060.980	0.194

0	1	27	6	21	27	7	21	21881.570	-0.400
0	1	28	6	22	28	7	22	17917.830	0.048
0	1	29	6	23	29	7	23	14292.040	0.207
0	1	29	7	22	29	8	22	34484.090	-0.622
0	1	31	7	24	31	8	24	25304.750	-0.402
0	1	32	7	25	32	8	25	20831.030	0.043
0	1	33	7	26	33	8	26	16695.540	0.197
0	1	34	7	27	34	8	27	13061.050	0.216
0	1	35	8	27	35	9	27	28888.080	-0.229
0	1	36	8	28	36	9	28	23915.450	0.110
0	1	37	8	29	37	9	29	19272.200	0.260
0	1	38	8	30	38	9	30	15140.900	0.164
0	1	39	9	30	39	10	30	32628.450	-0.297
0	1	40	9	31	40	10	31	27169.550	0.196
0	1	41	9	32	41	10	32	22022.160	0.303
0	1	42	9	33	42	10	33	17388.860	0.096
0	1	43	9	34	43	10	34	13418.880	0.119
0	1	43	10	33	43	11	33	36522.730	-0.305
0	1	44	10	34	44	11	34	30591.150	0.183
0	1	45	10	35	45	11	35	24945.150	0.293
0	1	46	10	36	46	11	36	19806.920	0.166
0	1	47	10	37	47	11	37	15347.970	-0.116
0	1	48	11	37	48	12	37	34177.650	0.091
0	1	49	11	38	49	12	38	28040.420	0.224
0	1	50	11	39	50	12	39	22396.150	0.062
0	1	51	11	40	51	12	40	17439.320	-0.064
0	1	52	11	41	52	12	41	13288.370	-0.298
0	1	52	12	40	52	13	40	37926.100	0.130
0	1	53	12	41	53	13	41	31306.770	0.173
0	1	54	12	42	54	13	42	25157.730	0.097
0	1	55	12	43	55	13	43	19695.640	-0.059
0	1	56	12	44	56	13	44	15064.320	-0.118
0	1	57	12	45	57	13	45	11314.700	0.152
0	1	57	13	44	57	14	44	34742.300	0.059
0	1	58	13	45	58	14	45	28091.820	0.112
0	1	59	13	46	59	14	46	22119.610	0.045
0	1	60	13	47	60	14	47	16995.130	0.280
0	1	61	14	47	61	15	47	38344.580	-0.184
0	1	62	14	48	62	15	48	31198.260	0.196
0	1	66	15	51	66	16	51	34475.920	0.048
1	0	2	2	0	3	3	0	32306.870	0.082
1	0	2	2	1	3	3	1	32358.220	0.056
1	0	3	1	2	4	2	2	29475.620	-0.265
1	0	3	1	3	4	2	3	31819.110	0.502
1	0	3	2	1	4	3	1	37566.280	0.016
1	0	4	1	4	5	2	4	38195.830	0.174
1	0	8	2	6	9	1	8	34569.120	0.044
1	0	8	3	5	9	2	7	33299.340	0.098
1	0	9	3	6	10	2	8	39296.620	0.122
1	0	10	3	7	10	4	7	19641.630	-0.194
1	0	10	4	6	10	5	6	30048.550	-0.079
1	0	11	3	8	11	4	8	17786.920	-0.019
1	0	12	3	9	12	4	9	15605.250	0.097
1	0	13	3	10	13	4	10	13194.180	0.061
1	0	13	4	9	13	5	9	27063.590	0.002
1	0	13	5	8	13	6	8	37229.110	0.275
1	0	14	4	10	14	5	10	25222.320	-0.032
1	0	14	5	9	14	6	9	36648.940	-0.119
1	0	15	3	13	15	4	11	38068.240	0.177
1	0	15	4	11	15	5	11	22931.080	-0.059
1	0	15	5	10	15	6	10	35803.440	-0.098
1	0	16	4	12	16	5	12	20260.180	0.067
1	0	16	4	12	16	5	12	20260.180	0.067
1	0	16	5	11	16	6	11	34596.200	-0.316
1	0	17	4	13	17	5	13	17320.420	0.117
1	0	17	4	13	17	5	13	17320.420	0.117
1	0	17	5	12	17	6	12	32936.950	-0.131
1	0	18	4	14	18	5	14	14246.080	0.081
1	0	18	5	13	18	6	13	30768.930	-0.335
1	0	19	4	15	19	5	15	11184.450	0.036
1	0	19	5	14	19	6	14	28097.300	-0.145
1	0	21	5	16	21	6	16	21569.260	0.090
1	0	22	5	17	22	6	17	17981.000	0.041
1	0	22	6	16	22	7	16	36313.430	-0.441
1	0	23	5	18	23	6	18	14390.800	0.067
1	0	23	6	17	23	7	17	33307.850	-0.262

1	0	24	6	18	24	7	18	29811.790	-0.030
1	0	25	6	19	25	7	19	25948.130	-0.017
1	0	26	6	20	26	7	20	21877.580	0.051
1	0	27	6	21	27	7	21	17779.810	0.108
1	0	27	7	20	27	8	20	38573.480	-0.313
1	0	28	6	22	28	7	22	13840.330	-0.058
1	0	28	7	21	28	8	21	34728.040	-0.007
1	0	29	7	22	29	8	22	30458.910	-0.040
1	0	30	7	23	30	8	23	25935.220	0.032
1	0	31	7	24	31	8	24	21349.950	-0.037
1	0	32	7	25	32	8	25	16904.990	-0.058
1	0	32	8	24	32	9	24	39740.310	-0.107
1	0	33	7	26	33	8	26	12793.960	-0.183
1	0	33	8	25	33	9	25	35099.940	-0.017
1	0	34	8	26	34	9	26	30151.210	-0.018
1	0	35	8	27	35	9	27	25098.830	-0.072
1	0	36	8	28	36	9	28	20159.570	-0.097
1	0	37	8	29	37	9	29	15544.570	-0.096
1	0	38	8	30	38	9	30	11436.750	-0.072
1	0	38	9	29	38	10	29	34521.440	0.013
1	0	40	9	31	40	10	31	23601.620	-0.097
1	0	41	9	32	41	10	32	18486.320	-0.098
1	0	42	9	33	42	10	33	13879.530	-0.066
1	0	43	10	33	43	11	33	33116.760	-0.002
1	0	44	10	34	44	11	34	27227.860	-0.084
1	0	45	10	35	45	11	35	21617.930	-0.066
1	0	46	10	36	46	11	36	16509.130	-0.083
1	0	47	10	37	47	11	37	12073.930	-0.097
1	0	47	11	36	47	12	36	37375.740	0.068
1	0	48	11	37	48	12	37	31034.380	-0.023
1	0	49	11	38	49	12	38	24937.130	-0.223
1	0	50	11	39	50	12	39	19325.770	-0.020
1	0	51	11	40	51	12	40	14394.610	-0.257
1	0	52	12	40	52	13	40	35016.660	0.180
1	0	53	12	41	53	13	41	28441.940	0.156
1	0	53	12	41	53	13	41	28441.940	0.156
1	0	54	12	42	54	13	42	22328.490	-0.311
1	0	55	12	43	55	13	43	16894.630	-0.505
1	0	56	13	43	56	14	43	39169.480	0.556
1	0	57	13	44	57	14	44	32128.090	0.167
1	0	58	13	45	58	14	45	25516.740	-0.320
1	0	61	14	47	61	15	47	35992.100	0.344
1	0	65	14	51	65	15	51	12184.660	-0.048
1	0	66	15	51	66	16	51	32440.760	-0.437
1	1	2	0	2	3	1	3	18220.110	-0.417
1	1	4	0	4	5	1	5	26999.540	-0.556
1	1	4	1	4	5	0	5	24053.390	0.256
1	1	5	0	5	6	1	6	31388.110	-0.520
1	1	5	1	5	6	0	6	29432.500	0.263
1	1	6	1	5	7	2	6	43256.130	-0.444
1	1	6	1	6	7	0	7	34645.690	0.176
1	1	7	0	7	8	1	8	40454.430	0.011
1	1	7	1	7	8	0	8	39724.030	0.327
1	1	8	1	8	9	0	9	44705.340	-0.291
1	1	8	2	7	9	1	8	44647.720	0.369
1	1	9	1	8	10	2	9	54831.370	-0.010
1	1	9	1	9	9	2	8	23377.780	-0.391
1	1	10	0	10	10	1	9	24270.030	-0.142
1	1	10	1	9	10	2	8	16034.720	-0.191
1	1	10	1	9	11	2	10	58940.290	0.074
1	1	10	1	10	10	2	9	25914.900	-0.248
1	1	10	1	10	11	0	11	54504.920	-0.035
1	1	10	2	9	11	1	10	56106.430	0.105
1	1	11	1	10	11	2	9	19129.710	-0.320
1	1	11	1	11	11	2	10	28575.090	-0.208
1	1	11	1	11	12	0	12	59362.440	0.067
1	1	12	0	12	12	1	11	30668.740	-0.036
1	1	12	1	11	12	2	10	22565.810	-0.195
1	1	12	1	12	12	2	11	31323.800	-0.109
1	1	12	2	11	12	3	10	27635.180	-0.612
1	1	13	0	13	13	1	12	33739.600	-0.002
1	1	13	1	12	13	2	11	26153.980	-0.274
1	1	13	1	13	13	2	12	34132.790	0.210
1	1	13	2	11	13	3	10	17608.000	-0.186
1	1	13	2	12	13	3	11	29909.680	-0.443
1	1	13	3	10	13	4	9	18944.030	-0.085

1	1	14	1	13	14	2	12	29737.660	-0.211
1	1	14	1	14	14	2	13	36979.930	0.137
1	1	14	2	12	14	3	11	20231.110	-0.129
1	1	14	2	13	14	3	12	32374.020	-0.304
1	1	14	3	11	14	4	10	18496.810	-0.375
1	1	14	3	12	14	4	11	30255.290	0.054
1	1	14	4	10	14	5	9	28217.570	0.371
1	1	15	1	14	15	2	13	33222.570	-0.078
1	1	15	2	13	15	3	12	23448.180	-0.214
1	1	15	2	14	15	3	13	34988.520	0.311
1	1	15	3	12	15	4	11	18720.120	-0.103
1	1	15	4	11	15	5	10	26589.810	0.239
1	1	16	1	15	16	2	14	36576.580	-0.066
1	1	16	2	14	16	3	13	27077.360	-0.196
1	1	16	3	13	16	4	12	19720.840	-0.024
1	1	16	3	14	16	4	13	33877.420	-0.669
1	1	16	4	12	16	5	11	25000.630	0.171
1	1	17	2	15	17	3	14	30908.390	-0.150
1	1	17	3	15	17	4	14	36076.390	-0.370
1	1	17	4	13	17	5	12	23696.540	0.057
1	1	18	2	16	18	3	15	34755.410	-0.123
1	1	18	3	15	18	4	14	24163.920	-0.131
1	1	18	3	16	18	4	15	38487.380	-0.300
1	1	18	4	14	18	5	13	22917.750	-0.026
1	1	19	2	17	19	3	16	38495.390	0.016
1	1	19	3	16	19	4	15	27465.000	-0.096
1	1	19	4	15	19	5	14	22857.530	-0.033
1	1	19	5	14	19	6	13	32004.680	0.314
1	1	20	3	17	20	4	16	31257.530	-0.128
1	1	20	4	16	20	5	15	23643.840	-0.031
1	1	20	5	15	20	6	14	30090.160	0.164
1	1	21	3	18	21	4	17	35312.930	-0.163
1	1	21	4	17	21	5	16	25334.250	-0.039
1	1	21	5	16	21	6	15	28443.210	-0.010
1	1	22	3	19	22	4	18	39418.120	0.018
1	1	22	4	18	22	5	17	27907.530	0.012
1	1	22	5	17	22	6	16	27327.910	0.016
1	1	23	4	19	23	5	18	31252.810	0.043
1	1	24	4	20	24	5	19	35175.670	0.045
1	1	24	5	19	24	6	18	27505.710	0.076
1	1	25	4	21	25	5	20	39432.670	0.177
1	1	25	6	19	25	7	18	33208.630	0.048
1	1	26	5	21	26	6	20	31511.010	0.113
1	1	26	6	20	26	7	19	31753.450	0.020
1	1	27	5	22	27	6	21	34860.800	0.152
1	1	27	5	22	27	6	21	34860.800	0.152
1	1	27	6	21	27	7	20	31070.660	0.038
1	1	28	5	23	28	6	22	38879.390	0.322
1	1	28	6	22	28	7	21	31338.240	0.199
1	1	29	6	23	29	7	22	32650.170	0.185
1	1	29	7	22	29	8	21	38008.180	0.075
1	1	30	6	24	30	7	23	35010.820	0.285
1	1	30	7	23	30	8	22	36212.290	0.061
1	1	31	6	25	31	7	24	38325.810	0.253
1	1	31	7	24	31	8	23	35196.250	0.196
1	1	32	7	25	32	8	24	35165.580	0.284
1	1	33	7	26	33	8	25	36238.090	0.417
1	1	34	7	27	34	8	26	38435.590	0.415
1	1	35	8	27	35	9	26	39357.320	0.264
1	1	36	8	28	36	9	27	39006.900	0.284
1	1	37	8	29	37	9	28	39810.050	0.561

RMS= 0.244 GRAMDET.=0.53E-49

ROTATIONAL CONSTANTS FOR LOWER STATE:

6385.405628	2937.541764	2415.081137
+- 0.008398	0.006074	0.006851

ROTATIONAL CONSTANTS FOR UPPER STATE:

6385.301674	2937.538380	2415.079232
0.009583	0.006161	0.007168

ENERGY DIFFERENCE BETWEEN COUPLING STATES AND COUPLING CONSTANTS IN MHZ:

DELTA-W	G -A	G -B	G -C	MU -AB	MU -BC	MU -CA
2280.1840	0.0000	0.0000	0.0000	0.0000	0.0000	39.8183
+- 0.0598	0.0000	0.0000	0.0000	0.0000	0.0000	0.1909

QUARTIC DISTORTION CONSTANTS:

	0.28560806	1.56123449	5.12609503	0.04938137	-0.13464263
+-	0.03031651	0.03130987	0.24332880	0.00101286	0.02458797
	0.25378116	2.62422450	-3.17077465	0.06431842	-0.38266315
+-	0.03042166	0.04316552	0.34844098	0.00131303	0.03346032

SIGNIFICANT DIGITS AND CORRELATION:

```

9.000
0.706 10.000
0.305 0.599 10.000
0.529 0.778 0.168 9.000
0.472 0.740 0.977 0.329 10.000
0.243 0.554 0.990 0.128 0.958 10.000
0.267 -0.097 -0.047 -0.333 -0.049 -0.067 7.000
-0.383 -0.335 0.544 -0.569 0.378 0.594 0.009 7.000
0.566 0.857 0.769 0.524 0.845 0.734 -0.072 0.002 7.000
-0.164 0.038 -0.047 0.298 -0.027 0.001 -0.188 -0.006 -0.043 6.000
0.282 -0.085 0.075 -0.343 0.059 0.026 0.254 0.098 0.021 -0.943 6.000
-0.204 -0.085 0.147 0.111 0.121 0.205 -0.233 0.353 -0.042 0.822 -0.668 6.000
0.119 0.030 -0.064 -0.149 -0.064 -0.099 0.216 -0.175 0.034 -0.747 0.595 -0.938 5.000
0.521 0.848 0.785 0.526 0.854 0.758 -0.097 0.038 0.997 0.007 -0.035 0.008 0.001 7.000
0.331 -0.106 0.073 -0.259 0.082 0.022 0.194 0.159 -0.022 -0.238 0.452 0.047 -0.176 -0.077 7.000
-0.241 0.161 -0.169 0.428 -0.141 -0.125 -0.242 -0.314 0.009 0.357 -0.538 0.07 3 0.023 0.062 -0.961
0.557 0.098 -0.266 0.135 -0.154 -0.338 0.209 -0.443 -0.037 -0.041 0.237 -0.012 -0.208 -0.101 0.760
-0.517 -0.131 0.300 -0.170 0.183 0.364 -0.193 0.514 0.031 -0.043 -0.130 -0.032 0.288 0.091 -0.658

6.000
-0.602 6.000
0.494 -0.974 6.000

```

Table 3S: Microwave Spectrum of the *Syn* 1 conformer of 1-Ethenylcyclopropan-1-ol (deuterated species)

CALCULATION BY ASMIX.

D1 = DJ, D2 = DJK, D3 = DK, D4 = SDJ, D5 = SDJK, (KHZ)
 D6 = HJ, D7 = HJK, D8 = HKJ, D9 = HK,
 D10 = SHJ, D11 = SHJK, D12 = SHK, (HZ).

TOTAL NUMBER OF ACCEPTED TRANSITIONS: 160

FIXED CONSTANTS:

G- A = 0.000000
 G- B = 0.000000
 G- C = 0.000000
 MU -AB = 0.000000
 MU -BC = 0.000000
 D6 -LOWER = 0.00000000
 D7 -LOWER = 0.00000000
 D8 -LOWER = 0.00000000
 D9 -LOWER = 0.00000000
 D10-LOWER = 0.00000000
 D11-LOWER = 0.00000000
 D12-LOWER = 0.00000000
 D6 -UPPER = 0.00000000
 D7 -UPPER = 0.00000000
 D8 -UPPER = 0.00000000
 D9 -UPPER = 0.00000000
 D10-UPPER = 0.00000000
 D11-UPPER = 0.00000000
 D12-UPPER = 0.00000000

ACCURACY: ± 0.10 MHZ

LABEL OF 0+ STATE: 0; LABEL OF 0- STATE: 1

		TRANSITION				OBS.FREQ.		OBS.- CALC.
VIB. ST.		J'K-'K+'		J''K+'K-''				
0 0	18 5 13	18 6 12	29567.920	-0.011				
0 0	22 6 16	22 7 15	34064.310	-0.018				
0 0	23 6 17	23 7 16	31925.760	-0.020				
0 0	24 6 18	24 7 17	30156.550	0.029				
0 0	28 6 22	28 7 21	31751.520	0.065				
0 0	28 7 21	28 8 20	34082.230	-0.009				
0 0	32 8 24	32 9 23	37936.510	-0.108				
0 0	33 8 25	33 9 24	36557.160	0.083				
0 1	2 1 2	3 2 2	27163.420	-0.049				
0 1	2 2 1	3 3 1	33284.690	0.025				
0 1	3 0 3	4 1 3	27609.230	-0.256				
0 1	3 1 2	4 2 2	30915.540	0.005				
0 1	3 1 3	4 2 3	33276.760	-0.053				
0 1	3 2 1	4 3 1	38421.200	-0.028				
0 1	3 2 2	4 3 2	38705.840	0.199				
0 1	4 1 4	5 2 4	39648.470	0.041				
0 1	6 4 3	6 5 1	30951.030	0.098				
0 1	7 4 4	7 5 2	30872.980	-0.022				
0 1	8 2 6	9 1 8	36153.320	0.011				
0 1	8 4 4	8 5 4	30630.530	-0.151				
0 1	8 4 5	8 5 3	30775.610	0.061				
0 1	9 4 5	9 5 5	30306.360	0.118				
0 1	9 4 6	9 5 4	30674.820	0.033				
0 1	9 5 4	9 6 4	37650.540	-0.034				
0 1	9 5 5	9 6 3	37666.930	-0.137				
0 1	10 3 8	10 4 6	25718.730	0.039				
0 1	10 4 7	10 5 5	30605.510	0.039				
0 1	10 5 6	10 6 4	37534.890	-0.083				
0 1	11 3 9	11 4 7	27209.900	0.130				
0 1	11 4 8	11 5 6	30627.820	0.008				
0 1	11 5 7	11 6 5	37373.160	0.080				
0 1	12 3 10	12 4 8	29487.720	0.063				
0 1	12 4 9	12 5 7	30834.080	0.028				
0 1	12 5 7	12 6 7	36888.330	-0.021				

0	1	12	5	8	12	6	6	37191.340	-0.005
0	1	13	3	11	13	4	9	32696.340	0.048
0	1	13	4	9	13	5	9	25975.920	-0.130
0	1	13	4	10	13	5	8	31353.410	0.007
0	1	13	5	9	13	6	7	37013.430	0.032
0	1	14	3	12	14	4	10	36897.150	0.028
0	1	14	4	11	14	5	9	32352.070	-0.103
0	1	14	5	10	14	6	8	36882.790	-0.027
0	1	15	4	12	15	5	10	34022.880	0.076
0	1	15	5	10	15	6	10	34408.530	-0.137
0	1	16	5	11	16	6	11	32786.350	0.158
0	1	16	5	12	16	6	10	37078.130	0.034
0	1	17	5	12	17	6	12	30632.590	-0.055
0	1	17	5	13	17	6	11	37648.490	0.115
0	1	18	5	13	18	6	13	27953.390	-0.274
0	1	18	5	14	18	6	12	38758.190	0.107
0	1	19	6	13	19	7	13	39658.010	-0.047
0	1	21	6	15	21	7	15	35104.650	-0.123
0	1	22	6	16	22	7	16	31968.010	-0.049
0	1	23	6	17	23	7	17	28356.190	0.016
0	1	25	7	18	25	8	18	39427.930	-0.139
0	1	26	7	19	26	8	19	35852.560	-0.053
0	1	27	7	20	27	8	20	31772.800	0.051
0	1	28	7	21	28	8	21	27358.670	0.143
0	1	30	8	22	30	9	22	39628.350	0.163
0	1	31	8	23	31	9	23	35097.300	0.111
0	1	32	8	24	32	9	24	30218.930	-0.036
0	1	33	8	25	33	9	25	25218.310	0.178
0	1	35	9	26	35	10	26	38341.520	-0.041
0	1	36	9	27	36	10	27	33013.840	-0.097
0	1	37	9	28	37	10	28	27568.020	0.109
0	1	40	10	30	40	11	30	35750.110	-0.064
0	1	41	10	31	41	11	31	29871.390	0.050
0	1	44	11	33	44	12	33	38432.720	0.001
0	1	45	11	34	45	12	34	32131.900	0.007
0	1	46	11	35	46	12	35	26008.950	-0.054
0	1	49	12	37	49	13	37	34352.160	0.005
0	1	50	12	38	50	13	38	27836.080	0.044
0	1	53	13	40	53	14	40	36534.020	-0.012
0	1	54	13	41	54	14	41	29633.020	-0.023
0	1	57	14	43	57	15	43	38678.860	-0.046
0	1	58	14	44	58	15	44	31400.660	-0.051
0	1	62	15	47	62	16	47	33139.510	0.079
0	1	63	15	48	63	16	48	26069.690	-0.090
0	1	66	16	50	66	17	50	34849.400	0.052
0	1	67	16	51	67	17	51	27446.620	0.003
1	0	2	1	2	3	2	2	27018.810	-0.067
1	0	2	2	0	3	3	0	33080.100	-0.052
1	0	3	1	2	4	2	2	30771.200	-0.069
1	0	3	2	1	4	3	1	38276.630	-0.227
1	0	3	2	2	4	3	2	38561.130	-0.115
1	0	4	0	4	5	1	4	34401.400	-0.012
1	0	4	1	3	5	2	3	36069.200	-0.182
1	0	4	1	4	5	2	4	39504.070	-0.076
1	0	6	4	2	6	5	2	30793.290	-0.064
1	0	6	4	3	6	5	1	30806.730	-0.039
1	0	7	2	5	8	1	7	32852.130	0.085
1	0	8	2	6	9	1	8	36011.070	0.264
1	0	9	2	7	10	1	9	38406.780	0.103
1	0	9	4	5	10	3	7	33950.720	0.146
1	0	9	4	6	9	5	4	30532.280	0.013
1	0	9	5	5	9	6	3	37523.760	-0.060
1	0	10	4	6	10	5	6	29633.020	-0.074
1	0	10	5	5	10	6	5	37343.570	-0.003
1	0	11	3	9	11	4	7	27068.940	0.189
1	0	11	4	7	11	5	7	28797.230	0.007
1	0	11	5	6	11	6	6	37103.300	-0.022
1	0	12	3	10	12	4	8	29347.280	-0.057
1	0	12	4	8	12	5	8	27554.920	0.219
1	0	12	4	9	12	5	7	30693.840	0.134
1	0	12	5	7	12	6	7	36747.530	-0.021
1	0	12	5	8	12	6	6	37050.480	-0.029
1	0	13	3	11	13	4	9	32556.660	-0.038
1	0	13	4	10	13	5	8	31214.020	0.134
1	0	13	5	8	13	6	8	36216.540	0.027
1	0	14	3	12	14	4	10	36758.220	-0.032

1	0	14	4	11	14	5	9	32213.500	-0.036
1	0	14	7	8	15	6	10	36842.870	-0.126
1	0	15	4	12	15	5	10	33885.020	-0.074
1	0	15	5	10	15	6	10	34271.140	0.129
1	0	16	4	13	16	5	11	36418.100	0.028
1	0	16	5	12	16	6	10	36941.350	0.100
1	0	17	4	14	17	5	12	39954.370	0.017
1	0	17	5	12	17	6	12	30497.470	-0.045
1	0	17	5	13	17	6	11	37512.670	0.027
1	0	18	5	13	18	6	13	27819.840	-0.037
1	0	18	5	14	18	6	12	38623.540	0.031
1	0	19	6	13	19	7	13	39525.030	0.294
1	0	21	6	15	21	7	15	34974.630	-0.015
1	0	22	6	16	22	7	16	31839.510	-0.081
1	0	23	6	17	23	7	17	28229.360	0.010
1	0	25	7	18	25	8	18	39303.720	-0.213
1	0	26	7	19	26	8	19	35730.220	-0.226
1	0	27	7	20	27	8	20	31652.480	-0.030
1	0	28	7	21	28	8	21	27240.140	0.021
1	0	30	8	22	30	9	22	39513.250	0.005
1	0	31	8	23	31	9	23	34984.490	0.042
1	0	32	8	24	32	9	24	30108.320	0.026
1	0	33	8	25	33	9	25	25109.390	0.054
1	0	35	9	26	35	10	26	38237.130	-0.028
1	0	36	9	27	36	10	27	32911.910	0.083
1	0	37	9	28	37	10	28	27467.930	0.071
1	0	40	10	30	40	11	30	35657.280	-0.089
1	0	41	10	31	41	11	31	29780.850	0.092
1	0	44	11	33	44	12	33	38349.940	0.064
1	0	45	11	34	45	12	34	32051.440	0.021
1	0	46	11	35	46	12	35	25930.520	0.018
1	0	49	12	37	49	13	37	34282.320	-0.009
1	0	50	12	38	50	13	38	27768.300	0.032
1	0	53	13	40	53	14	40	36475.260	-0.037
1	0	54	13	41	54	14	41	29576.400	-0.036
1	0	57	14	43	57	15	43	38631.540	-0.063
1	0	58	14	44	58	15	44	31355.560	-0.032
1	0	62	15	47	62	16	47	33106.070	0.043
1	0	63	15	48	63	16	48	26037.920	-0.039
1	0	66	16	50	66	17	50	34827.830	0.041
1	0	67	16	51	67	17	51	27426.630	-0.020
1	0	70	17	53	70	18	53	36520.740	0.017
1	1	18	5	13	18	6	12	29568.570	-0.003
1	1	22	6	16	22	7	15	34065.260	0.067
1	1	23	6	17	23	7	16	31926.620	0.020
1	1	24	6	18	24	7	17	30157.170	-0.001
1	1	28	6	22	28	7	21	31750.090	-0.049
1	1	28	7	21	28	8	20	34083.070	-0.005
1	1	32	8	24	32	9	23	37937.610	-0.042
1	1	33	8	25	33	9	24	36557.580	-0.097

RMS= 0.096 GRAMDET.=0.24E-58

ROTATIONAL CONSTANTS FOR LOWER STATE:

6104.361638	2926.088514	2378.912395
0.005029	0.002736	0.003966

ROTATIONAL CONSTANTS FOR UPPER STATE:

6104.344850	2926.065483	2378.910415
0.005420	0.002733	0.003969

ENERGY DIFFERENCE BETWEEN COUPLING STATES AND COUPLING CONSTANTS IN MHZ:

DELTA-W	G -A	G -B	G -C	MU -AB	MU -BC	MU -CA
72.4008	0.0000	0.0000	0.0000	0.0000	0.0000	5.2481
0.0269	0.0000	0.0000	0.0000	0.0000	0.0000	1.0278

QUARTIC DISTORTION CONSTANTS:

0.38549968	2.00422569	1.08038448	0.04696430	0.14356661
0.01283164	0.03218072	0.13348307	0.00182993	0.05012245
0.35474969	2.31925913	-0.10637112	0.06164460	-0.24709908
0.01218396	0.02944298	0.12194460	0.00172459	0.04730346

SIGNIFICANT DIGITS AND CORRELATION:

```

10.000
0.532 11.000
-0.119 0.639 10.000
0.613 0.551 -0.095 10.000
0.519 0.993 0.674 0.521 11.000
-0.062 0.631 0.970 -0.169 0.650 10.000
0.122 0.044 0.278 -0.407 0.103 0.277 6.000
-0.548 -0.066 0.700 -0.623 -0.031 0.719 0.297 5.000
0.450 0.749 0.302 0.691 0.728 0.256 -0.164 -0.297 8.000
-0.634 -0.086 0.521 -0.493 -0.038 0.465 0.181 0.659 -0.317 7.000
0.673 -0.005 -0.311 0.131 -0.017 -0.202 0.145 -0.258 0.033 -0.770 6.000
-0.527 -0.115 0.541 -0.608 -0.059 0.528 0.286 0.755 -0.408 0.942 -0.523 7.000
0.540 0.108 -0.540 0.622 0.051 -0.524 -0.294 -0.739 0.401 -0.936 0.530 -0.995 6.000
0.239 0.744 0.625 0.432 0.754 0.572 -0.009 0.122 0.867 0.094 -0.142 0.052 -0.051 8.000
0.276 -0.019 -0.489 0.161 -0.061 -0.445 -0.119 -0.649 0.052 -0.432 0.126 -0.507 0.483 -0.366 7.000
-0.144 0.095 0.248 0.382 0.099 0.150 -0.246 0.246 0.274 0.106 -0.146 0.054 -0.027 0.439 -0.742
0.277 0.033 -0.504 0.387 -0.018 -0.503 -0.241 -0.729 0.214 -0.497 0.070 -0.628 0.601 -0.250 -0.938
-0.237 -0.042 0.482 -0.358 0.011 0.479 0.244 0.711 -0.215 0.472 -0.037 0.602 -0.567 0.240 -0.930

5.000
-0.478 7.000
0.482 -0.994 6.000

```

Table 4S: Microwave spectrum of the Ground Vibrational state of
1-Ethenylcyclopropan-1-ol Skew 1 Conformer

D1 = DJ, D2 = DJK, D3 = DK, D4 = SDJ, D5 = SDK, (KHZ)
D6 = HJ, D7 = HJK, D8 = HKJ, D9 = HK,
D10= SHJ, D11= SHJK, D12= SHK, (HZ).

TRANSITION						OBS.FREQ.	O.-C.	DISTORTION CONTRIBUTION
								TOTAL
5	4	1	6	4	2	34389.470	-0.084	-2.02
6	5	1	7	5	2	40040.550	0.018	-3.56
6	5	2	7	5	3	40033.930	0.020	-3.56
7	5	2	8	5	3	45876.770	-0.075	-4.39
7	5	3	8	5	4	45850.880	-0.246	-4.41
8	3	5	9	3	6	53801.390	0.187	-3.09
8	4	4	9	4	5	52578.530	-0.227	-3.77
8	6	2	9	6	3	51528.210	0.259	-6.85
8	6	2	9	6	3	51528.000	0.049	-6.85
8	6	3	9	6	4	51524.500	0.111	-6.85
8	7	1	9	7	2	51404.810	-0.010	-8.58
8	7	2	9	7	3	51404.810	0.073	-8.58
8	8	0	9	8	1	51327.120	0.103	-10.56
8	8	1	9	8	2	51327.120	0.104	-10.56
9	3	6	10	3	7	59813.610	-0.114	-4.33
9	3	7	10	3	8	56359.880	-0.061	-5.02
9	5	4	10	5	5	57774.320	0.097	-6.28
9	6	3	10	6	4	57374.640	0.097	-8.12
9	6	4	10	6	5	57361.540	-0.046	-8.14
9	9	0	10	9	1	57019.370	-0.139	-14.77
9	9	1	10	9	2	57019.370	-0.139	-14.77

STOPPED ON DIVERGENCY

RMS= 0.1468 GRAMDET.=0.21E-03

ROTATIONAL CONSTANTS (MHZ):

	5506.936177	3161.668415	2494.888909
+	0.231517	0.019454	0.020993

QUARTIC DISTORTION CONSTANTS:

	0.82290977	7.17943003	0.00000000	0.00000000	0.00000000
+	0.06081174	0.09890694	0.00000000	0.00000000	0.00000000

SIGNIFICANT DIGITS AND CORRELATION MATRIX:

13.000				
0.810	16.000			
-0.565	-0.480	15.000		
0.398	0.727	0.172	6.000	

-0.453 -0.456 0.542 -0.332 7.000

DERIVED CONSTANTS:

KAPPA=-0.557258

MOMENTS OF INERTIA AND DEFECT (U*A**2):

	91.77136501	159.84568388	202.56575277	-49.05129612
+	0.00385815	0.00098353	0.00170443	0.00582634

STANDARD DISTORTION CONSTANTS (KHZ):

-32.009359	-3.291639	-3.291639
-17.650499	-3.291639	-17.650499