Table S1. The observed and the obs.-calc. frequencies (MHz) of measured rotational transitions in the ground state of the parent isotopomer of camphor.

Camphor ground state, combined supersonic FTMW and room-temperature MMW

Obs-calc differences are from fit of Watson's reduced Hamiltonian in
---> reduction-A, representation-I.r <---

TRANSITION	Observed	Obs-Calc	Error
!			
! Supersonic expansion FTMW spectra			
!			
! a-type transitions			
!			
3, 1, 3 <- 2, 1, 2	6701.753	0.000	0.002
3, 0, 3 <- 2, 0, 2	6774.254	0.000	0.002
3, 1, 2 <- 2, 1, 1	6958.158	0.000	0.002
4, 1, 4 <- 3, 1, 3	8919.513	0.000	0.002
4, 0, 4 <- 3, 0, 3	8975.682	-0.002	0.002
4, 2, 3 <- 3, 2, 2	9107.764	0.001	0.002
4, 3, 2 <- 3, 3, 1	9151.676	0.000	0.002
4, 1, 3 <- 3, 1, 2	9250.655	-0.001	0.002
4, 2, 2 <- 3, 2, 1	9253.678	-0.002	0.002
5, 1, 5 <- 4, 1, 4	11128.703	0.000	0.002
5, 0, 5 <- 4, 0, 4	11162.935	-0.001	0.002
5, 2, 4 <- 4, 2, 3	11362.617	-0.001	0.002
5, 3, 3 <- 4, 3, 2	11443.138	0.000	0.002
5, 3, 2 <- 4, 3, 1	11488.682	-0.001	0.002
5, 1, 4 <- 4, 1, 3	11514.459	-0.001	0.002
5, 2, 3 <- 4, 2, 2	11599.937	-0.002	0.002
6, 1, 6 <- 5, 1, 5	13331.410	0.001	0.002
6, 0, 6 <- 5, 0, 5	13349.164	-0.001	0.002
6, 2, 5 <- 5, 2, 4	13604.411	-0.001	0.002
6, 3, 4 <- 5, 3, 3	13729.709	0.001	0.002
6, 4, 3 <- 5, 4, 2	13741.014	0.002	0.002
6, 1, 5 <- 5, 1, 4	13741.902	-0.001	0.002
6, 4, 2 <- 5, 4, 1	13749.988	-0.001	0.002
6, 3, 3 <- 5, 3, 2	13836.546	0.000	0.002
6, 2, 4 <- 5, 2, 3	13929.050	0.003	0.002
7, 1, 7 <- 6, 1, 6	15529.953	0.001	0.002
7, 0, 7 <- 6, 0, 6	15538.285	-0.002	0.002
7, 1, 6 <- 6, 1, 5	15937.009	0.000	0.002
7, 2, 6 <- 6, 2, 5	15833.025	0.000	0.002
7, 3, 5 <- 6, 3, 4	16006.993	0.000	0.002
7, 5, 3 <- 6, 5, 2	16027.668	0.000	0.002
7, 4, 4 <- 6, 4, 3	16042.196	0.000	0.002
7, 4, 3 <- 6, 4, 2	16070.315	0.002	0.002
7, 3, 4 <- 6, 3, 3	16202.403	0.000	0.002
7, 2, 5 <- 6, 2, 4	16229.825	0.001	0.002
8, 1, 8 <- 7, 1, 7	17726.167	0.002	0.002
8, 0, 8 <- 7, 0, 7	17729.837	-0.001	0.002
8, 2, 7 <- 7, 2, 6	18049.913	0.000	0.002
8, 1, 7 <- 7, 1, 6	18116.163	0.000	0.002

```
   8,  3,  6 <-  7,  3,  5        18271.529     0.000     0.002
   8,  4,  4 <-  7,  4,  3        18411.916     0.001     0.002
   8,  2,  6 <-  7,  2,  5        18493.913     0.000     0.002
!
!  b-type transitions
!
   4,  0,  4 <-  3,  1,  3         8852.917     0.001     0.002
   4,  1,  4 <-  3,  0,  3         9042.281     0.000     0.002
   4,  3,  2 <-  3,  2,  1        10610.517    -0.002     0.002
   4,  3,  1 <-  3,  2,  2        10711.909    -0.001     0.002
   5,  0,  5 <-  4,  1,  4        11096.337     0.000     0.002
   5,  1,  5 <-  4,  0,  4        11195.302     0.000     0.002
   4,  4,  0 <-  3,  3,  1        11273.114    -0.001     0.002
   5,  2,  4 <-  4,  1,  3        11893.772     0.001     0.002
   5,  3,  3 <-  4,  2,  2        12799.976     0.000     0.002
   5,  3,  2 <-  4,  2,  3        13092.830     0.000     0.002
   6,  0,  6 <-  5,  1,  5        13316.797    -0.001     0.002
   6,  1,  6 <-  5,  0,  5        13363.776     0.001     0.002
   5,  4,  2 <-  4,  3,  1        13546.874    -0.002     0.002
   5,  4,  1 <-  4,  3,  2        13565.521     0.002     0.002
   5,  5,  1 <-  4,  4,  0        14165.703     0.004     0.002
   7,  0,  7 <-  6,  1,  6        15523.677     0.002     0.002
   7,  1,  7 <-  6,  0,  6        15544.565     0.002     0.002
   6,  4,  3 <-  5,  3,  2        15799.206     0.000     0.002
   6,  4,  2 <-  5,  3,  3        15872.370    -0.001     0.002
!
!  c-type transitions
!
   4,  2,  2 <-  3,  1,  2        10012.805    -0.001     0.002
   4,  3,  1 <-  3,  2,  1        10626.829    -0.001     0.002
   4,  3,  2 <-  3,  2,  2        10695.597    -0.001     0.002
   5,  2,  3 <-  4,  1,  3        12362.091     0.002     0.002
   5,  3,  3 <-  4,  2,  3        13030.972    -0.002     0.003
   5,  4,  2 <-  4,  3,  2        13563.188     0.000     0.002
   5,  4,  1 <-  4,  3,  1        13549.209     0.002     0.002
!
!  Room-temperature MMW spectra
!
!  a-type transitions in order of increasing K-1
!
  84,  0, 84 <- 83,  0, 83       184420.458    -0.005     0.050
  85,  0, 85 <- 84,  0, 84       186612.268    -0.008     0.050
  89,  0, 89 <- 88,  0, 88       195379.026     0.071     0.050
  90,  0, 90 <- 89,  0, 89       197570.468    -0.010     0.050
  92,  0, 92 <- 91,  0, 91       201953.327    -0.016     0.050
  93,  0, 93 <- 92,  0, 92       204144.691     0.008     0.050
  94,  0, 94 <- 93,  0, 93       206335.936    -0.026     0.050
  97,  0, 97 <- 96,  0, 96       212909.417    -0.002     0.050
  98,  0, 98 <- 97,  0, 97       215100.473     0.031     0.050
 101,  0,101 <-100,  0,100       221673.121     0.003     0.050

  79,  1, 78 <- 78,  1, 77       173807.258     0.003     0.050
  84,  1, 83 <- 83,  1, 82       184766.981    -0.059     0.050
  88,  1, 87 <- 87,  1, 86       193533.909     0.051     0.050
  89,  1, 88 <- 88,  1, 87       195725.419     0.002     0.050
  90,  1, 89 <- 89,  1, 88       197916.901    -0.015     0.050
  94,  1, 93 <- 93,  1, 92       206682.316     0.013     0.050
  96,  1, 95 <- 95,  1, 94       211064.666     0.044     0.050

  79,  2, 77 <- 78,  2, 76       174153.985    -0.035     0.050
  84,  2, 82 <- 83,  2, 81       185113.747     0.062     0.050
  88,  2, 86 <- 87,  2, 85       193880.360    -0.044     0.050
  89,  2, 87 <- 88,  2, 86       196071.950     0.012     0.050
  96,  2, 94 <- 95,  2, 93       211410.986     0.024     0.050
  98,  2, 96 <- 97,  2, 95       215792.978     0.009     0.050
```

100,	2,	98	<-	99,	2,	97		220174.734	0.020	0.050
84,	3,	81	<-	83,	3,	80		185460.483	0.028	0.050
88,	3,	85	<-	87,	3,	84		194226.986	-0.077	0.050
95,	3,	92	<-	94,	3,	91		209566.295	-0.026	0.050
96,	3,	93	<-	95,	3,	92		211757.410	0.017	0.050
79,	4,	75	<-	78,	4,	74		174848.028	-0.036	0.050
84,	4,	80	<-	83,	4,	79		185807.441	0.022	0.050
89,	4,	85	<-	88,	4,	84		196765.378	0.010	0.050
92,	4,	88	<-	91,	4,	87		203339.417	-0.008	0.050
93,	4,	89	<-	92,	4,	88		205530.646	-0.009	0.050
96,	4,	92	<-	95,	4,	91		212103.945	-0.020	0.050
84,	5,	79	<-	83,	5,	78		186154.642	-0.014	0.050
89,	5,	84	<-	88,	5,	83		197112.356	-0.047	0.050
93,	5,	88	<-	92,	5,	87		205877.433	-0.103	0.050
84,	6,	78	<-	83,	6,	77		186502.276	0.019	0.050
93,	6,	87	<-	92,	6,	86		206224.723	0.024	0.050
95,	6,	89	<-	94,	6,	88		210606.767	-0.038	0.050
78,	7,	71	<-	77,	7,	70		173699.939	-0.042	0.050
90,	7,	83	<-	89,	7,	82		199998.787	0.009	0.050
93,	7,	86	<-	92,	7,	85		206572.287	0.062	0.050
94,	7,	87	<-	93,	7,	86		208763.260	0.006	0.050
98,	7,	91	<-	97,	7,	90		217526.669	-0.075	0.050
83,	8,	75	<-	82,	8,	74		185007.470	-0.028	0.050
87,	8,	79	<-	86,	8,	78		193773.201	-0.030	0.050
78,	9,	69	<-	77,	9,	68		174399.382	-0.043	0.050
83,	9,	74	<-	82,	9,	73		185357.041	0.000	0.050
94,	9,	85	<-	93,	9,	84		209459.614	-0.014	0.050
95,	9,	86	<-	94,	9,	85		211650.547	0.101	0.050
78,	10,	68	<-	77,	10,	67		174750.767	-0.018	0.050
83,	10,	73	<-	82,	10,	72		185707.553	0.003	0.050
92,	10,	82	<-	91,	10,	81		205427.188	0.025	0.050
83,	11,	72	<-	82,	11,	71		186059.279	0.027	0.050
92,	11,	81	<-	91,	11,	80		205777.402	0.031	0.050
96,	11,	85	<-	95,	11,	84		214539.806	-0.013	0.050
82,	12,	70	<-	81,	12,	69		184221.534	-0.070	0.050
83,	12,	71	<-	82,	12,	70		186412.351	-0.069	0.050
90,	12,	79	<-	89,	12,	78		201395.880	0.025	0.050
92,	12,	80	<-	91,	12,	79		206128.666	0.041	0.050
87,	13,	74	<-	86,	13,	73		195529.190	-0.036	0.050
88,	13,	75	<-	87,	13,	74		197719.631	-0.024	0.050
92,	13,	79	<-	91,	13,	78		206481.112	-0.028	0.050
77,	14,	63	<-	76,	14,	62		173985.153	0.064	0.050
86,	14,	72	<-	85,	14,	71		193694.704	-0.041	0.050
82,	14,	69	<-	81,	14,	68		184576.925	0.010	0.050
87,	14,	73	<-	86,	14,	72		195884.830	0.003	0.050
89,	14,	75	<-	88,	14,	74		200264.964	-0.027	0.050
90,	14,	76	<-	89,	14,	75		202455.045	-0.019	0.050
92,	14,	78	<-	91,	14,	77		206835.107	-0.063	0.050
93,	14,	79	<-	92,	14,	78		209025.210	0.015	0.050
95,	14,	81	<-	94,	14,	80		213405.221	0.045	0.050
82,	15,	67	<-	81,	15,	66		185295.037	0.004	0.050
88,	15,	73	<-	87,	15,	72		198432.330	0.004	0.050

```
93, 15, 78 <- 92, 15, 77       209380.742     0.036     0.050
95, 15, 80 <- 94, 15, 79       213760.120     0.077     0.050
96, 15, 81 <- 95, 15, 80       215949.727     0.036     0.050

82, 16, 66 <- 81, 16, 65       185659.138     0.053     0.050
91, 16, 75 <- 90, 16, 74       205359.880     0.027     0.050
95, 16, 79 <- 94, 16, 78       214116.887     0.035     0.050

82, 17, 65 <- 81, 17, 64       186027.560    -0.045     0.050
87, 17, 70 <- 86, 17, 69       196967.250    -0.059     0.050
91, 17, 74 <- 90, 17, 73       205721.214     0.063     0.050
92, 17, 76 <- 91, 17, 75       207549.105     0.027     0.050
94, 17, 77 <- 93, 17, 76       212287.211    -0.009     0.050

81, 18, 63 <- 80, 18, 62       184215.859    -0.011     0.050
82, 18, 64 <- 81, 18, 63       186401.746    -0.050     0.050
87, 18, 69 <- 86, 18, 68       197335.540     0.029     0.050
91, 18, 73 <- 90, 18, 72       206085.853     0.007     0.050
93, 18, 75 <- 92, 18, 74       210461.753     0.027     0.050
94, 18, 76 <- 93, 18, 75       212649.776    -0.020     0.050
98, 18, 80 <- 97, 18, 79       221402.679    -0.016     0.050

81, 19, 62 <- 80, 19, 61       184599.365    -0.067     0.050
86, 19, 67 <- 85, 19, 66       195523.126    -0.013     0.050
87, 19, 68 <- 86, 19, 67       197709.028     0.065     0.050
91, 19, 72 <- 90, 19, 71       206454.660    -0.055     0.050
93, 19, 74 <- 92, 19, 73       210828.764     0.041     0.050

76, 20, 57 <- 75, 20, 56       173689.893    -0.013     0.050
81, 20, 61 <- 80, 20, 60       184993.412    -0.086     0.050
88, 20, 68 <- 87, 20, 67       200273.414    -0.061     0.050
89, 20, 69 <- 88, 20, 68       202458.246    -0.004     0.050
91, 20, 71 <- 90, 20, 70       206828.780     0.019     0.050
92, 20, 72 <- 91, 20, 71       209014.390    -0.041     0.050
94, 20, 74 <- 93, 20, 73       213386.495     0.035     0.050

76, 21, 55 <- 75, 21, 54       174551.608     0.110     0.050
76, 21, 56 <- 75, 21, 55       174103.739     0.069     0.050
92, 21, 71 <- 91, 21, 70       209393.284    -0.043     0.050
94, 21, 73 <- 93, 21, 72       213762.353    -0.035     0.050
95, 21, 74 <- 94, 21, 73       215947.366    -0.001     0.050
97, 21, 76 <- 96, 21, 75       220318.054    -0.021     0.050

76, 22, 55 <- 75, 22, 54       174538.905     0.108     0.050
90, 22, 68 <- 89, 22, 67       205416.994    -0.017     0.050
94, 22, 72 <- 93, 22, 71       214145.075    -0.022     0.050
95, 22, 73 <- 94, 22, 72       216328.298    -0.028     0.050
97, 22, 75 <- 96, 22, 74       220695.951     0.051     0.050

81, 23, 59 <- 80, 23, 58       185829.202     0.013     0.050
90, 23, 67 <- 89, 23, 66       205820.108    -0.073     0.050
91, 23, 68 <- 90, 23, 67       207997.934    -0.035     0.050
94, 23, 71 <- 93, 23, 70       214536.470     0.012     0.050
95, 23, 72 <- 94, 23, 71       216717.364     0.018     0.050
97, 23, 74 <- 96, 23, 73       221080.849     0.072     0.050

75, 24, 51 <- 74, 24, 50       174632.860    -0.092     0.050
86, 24, 62 <- 85, 24, 61       197571.755    -0.036     0.050
90, 24, 67 <- 89, 24, 66       205820.108     0.018     0.050
92, 24, 68 <- 91, 24, 67       210586.761    -0.095     0.050
95, 24, 71 <- 94, 24, 70       217116.770    -0.031     0.050

75, 25, 50 <- 74, 25, 49       174786.977    -0.058     0.050
80, 25, 56 <- 79, 25, 55       184570.320    -0.050     0.050
86, 25, 62 <- 85, 25, 61       197562.851    -0.017     0.050
```

```
  92, 25, 67 <- 91, 25, 66       211016.164    -0.007     0.050
  92, 25, 68 <- 91, 25, 67       210586.761     0.104     0.050
  95, 25, 70 <- 94, 25, 69       217530.175    -0.033     0.050

  75, 26, 49 <- 74, 26, 48       174128.490    -0.098     0.050
  84, 26, 59 <- 83, 26, 58       193701.891    -0.060     0.050
  90, 26, 65 <- 89, 26, 64       206679.341    -0.033     0.050
  92, 26, 67 <- 91, 26, 66       211014.642     0.007     0.050
  93, 26, 68 <- 92, 26, 67       213184.806    -0.094     0.050
  95, 26, 69 <- 94, 26, 68       217963.380    -0.057     0.050

  93, 27, 66 <- 92, 27, 65       214134.340     0.034     0.050
  93, 27, 67 <- 92, 27, 66       213629.530     0.087     0.050
  94, 27, 68 <- 93, 27, 67       215794.744     0.094     0.050
  95, 27, 69 <- 94, 27, 68       217961.860     0.100     0.050
  96, 27, 69 <- 95, 27, 68       220585.640     0.037     0.050

  92, 28, 64 <- 91, 28, 63       212693.454    -0.020     0.050
  93, 28, 66 <- 92, 28, 65       214099.433    -0.072     0.050
  94, 28, 67 <- 93, 28, 66       216257.904    -0.001     0.050
  96, 28, 69 <- 95, 28, 68       220579.477     0.046     0.050
  96, 28, 68 <- 95, 28, 67       221091.209    -0.023     0.050

  96, 29, 68 <- 95, 29, 67       221054.277     0.022     0.050
  96, 29, 67 <- 95, 29, 66       221723.856    -0.044     0.050

  93, 30, 63 <- 92, 30, 62       216637.468    -0.023     0.050
  96, 30, 67 <- 95, 30, 66       221539.911     0.080     0.050
!
!  high-K sequences for a given J
!
  76, 31, 46 <- 75, 31, 45       175020.931     0.039     0.050
  76, 33, 44 <- 75, 33, 43       174796.444    -0.010     0.050
  76, 35, 41 <- 75, 35, 40       174624.709     0.039     0.050
  76, 36, 40 <- 75, 36, 39       174552.600     0.053     0.050
  76, 39, 37 <- 75, 39, 36       174375.092    -0.031     0.050
  76, 41, 35 <- 75, 41, 34       174280.857    -0.065     0.050
  76, 44, 32 <- 75, 44, 31       174164.936    -0.044     0.050
  76, 45, 31 <- 75, 45, 30       174131.664     0.003     0.050
  76, 46, 30 <- 75, 46, 29       174100.560     0.005     0.050
  76, 47, 29 <- 75, 47, 28       174071.384    -0.060     0.050
  76, 48, 28 <- 75, 48, 27       174044.169     0.030     0.050
  76, 50, 26 <- 75, 50, 25       173994.312     0.015     0.050

  86, 38, 48 <- 85, 38, 47       197711.285    -0.029     0.050

  87, 36, 52 <- 86, 36, 51       200262.883     0.058     0.050

  93, 38, 56 <- 92, 38, 55       214118.315     0.094     0.050
  93, 43, 50 <- 92, 43, 49       213627.552     0.038     0.050
```

Table S2. The observed and the obs.-calc. frequencies (MHz) of measured rotational transitions in the ground states of singly substituted 13C and the 18O isotopomer of camphor.

	13C.1		13C.2		13C.3	
4 1 4 <- 3 1 3	8913.5934	0.0001	8882.4569	-0.0001	8877.0557	-0.0003
4 0 4 <- 3 0 3	8969.4788	-0.0005	8939.8532	0.0004	8931.6100	-0.0001
4 1 3 <- 3 1 2	9243.5572	-0.0006	9210.9904	-0.0011	9210.6792	0.0001
5 1 5 <- 4 1 4	11121.3622	0.0003	11082.8447	-0.0001	11075.1096	0.0001
5 0 5 <- 4 0 4	11155.3906	-0.0001	11118.4356	-0.0006	11107.6550	0.0002
5 2 4 <- 4 2 3			11314.4014	0.0010		
5 1 4 <- 4 1 3	11505.6837	0.0007	11466.7858	0.0004	11462.1930	-0.0001
5 2 3 <- 4 2 2						

	13C.4		13C.5		13C.6	
4 1 4 <- 3 1 3	8884.9285	0.0004	8857.1101	-0.0006	8902.9231	0.0000
4 0 4 <- 3 0 3	8939.7075	-0.0002	8910.0307	0.0002	8958.2303	-0.0005
4 1 3 <- 3 1 2	9223.8052	0.0001	9205.3622	-0.0008	9210.6284	-0.0005
5 1 5 <- 4 1 4	11084.5003	-0.0005	11048.5143	0.0014	11109.9860	0.0003
5 0 5 <- 4 0 4	11116.9647	0.0003	11078.7857	-0.0012	11144.8668	-0.0001
5 2 4 <- 4 2 3						
5 1 4 <- 4 1 3	11477.1778	-0.0001	11449.2445	0.0008	11470.6757	0.0006
5 2 3 <- 4 2 2						

	13C.7		13C.8		13C.9	
4 1 4 <- 3 1 3	8900.4646	-0.0018	8874.9098	-0.0011	8810.4628	-0.0010
4 0 4 <- 3 0 3	8957.0875	0.0012	8929.5507	-0.0001	8869.6392	-0.0004
4 1 3 <- 3 1 2	9229.5774	0.0008	9188.2048	0.0006	9138.5086	0.0000
5 1 5 <- 4 1 4	11105.1653	0.0011	11074.3342	0.0006	10993.2166	0.0009
5 0 5 <- 4 0 4	11139.9575	-0.0004	11108.1823	0.0004	11030.6167	0.0001
5 2 4 <- 4 2 3						
5 1 4 <- 4 1 3	11489.1410	-0.0009	11440.3952	-0.0005	11377.8924	0.0001
5 2 3 <- 4 2 2	11571.8250	0.0001				

	13C.10		18O	
4 1 4 <- 3 1 3	8851.7065	0.0008	8676.1001	0.0001
4 0 4 <- 3 0 3	8903.6811	-0.0014	8739.7319	0.0010
4 1 3 <- 3 1 2	9200.0693	-0.0013	8992.0243	-0.0012
5 1 5 <- 4 1 4	11041.5724	0.0003	10827.1650	0.0005
5 0 5 <- 4 0 4	11071.0013	-0.0002	10870.1739	-0.0015
5 2 4 <- 4 2 3				
5 1 4 <- 4 1 3	11441.5918	0.0015	11201.8184	0.0010
5 2 3 <- 4 2 2				

Table S3. The results of fitting the r0 geometry of the camphor molecule.

CAMPHOR, standard bond type declaration starting at the oxygen

---

```
!
!  CH bonds from [MP2+(1/4)(MP2-HF)]/6-31G** rounded to nearest 0.001A
!
```

NUMBER OF ATOMS = 27

NO	NA	NB	NC	NO.NA	NO.NA.NB	NO.NA.NB.NC	MASS	Fig.1
1	0	0	0	0.000000	0.000000	0.000000	15.9949150	= O
2	1	0	0	1.225510	0.000000	0.000000	12.0000000	= C2
3	2	1	0	1.527410	126.634000	0.000000	12.0000000	= C1
4	2	1	3	1.535990	126.648000	-179.703000	12.0000000	= C3
5	3	2	1	1.513010	113.903000	16.919000	12.0000000	= C10
6	4	2	5	1.537890	101.432000	-13.656000	12.0000000	= C4
7	3	2	1	1.557260	100.279000	145.912000	12.0000000	= C7
8	3	2	4	1.555860	103.308000	70.849000	12.0000000	= C6
9	6	4	2	1.542350	106.544000	-72.288000	12.0000000	= C5
10	7	3	5	1.529750	114.152000	-63.350000	12.0000000	= C9
11	7	3	5	1.532870	112.976000	60.464000	12.0000000	= C8
12	5	3	7	1.091000	109.923000	-175.885000	1.0078250	= H10
13	5	3	7	1.092000	111.058000	-57.139000	1.0078250	= H10′
14	5	3	7	1.091000	111.020000	63.929000	1.0078250	= H10′′
15	6	7	3	1.094000	114.822000	179.918000	1.0078250	= H4
16	4	2	1	1.093000	109.684000	-60.094000	1.0078250	= H3
17	4	2	1	1.093000	110.784000	58.298000	1.0078250	= H3′
18	9	8	3	1.092000	111.577000	-117.360000	1.0078250	= H5
19	9	8	3	1.092000	112.432000	122.331000	1.0078250	= H5′
20	8	9	6	1.093000	112.976000	-118.360000	1.0078250	= H8
21	8	9	6	1.093000	111.963000	120.812000	1.0078250	= H8′
22	10	7	3	1.093000	109.716000	-172.169000	1.0078250	= H9
23	10	7	3	1.092000	110.291000	69.501000	1.0078250	= H9′
24	10	7	3	1.089000	113.430000	-51.530000	1.0078250	= H9′′
25	11	7	3	1.092000	110.113000	-73.539000	1.0078250	= H8
26	11	7	3	1.091000	110.221000	167.908000	1.0078250	= H8′
27	11	7	3	1.091000	113.378000	46.667000	1.0078250	= H8′′

FINAL RESULTS OF LEAST SQUARES FIT:

```
          R( 3, 2) =     1.537218 +-  0.010057
          R( 8, 3) =     1.556614 +-  0.006475
          R( 7, 3) =     1.543110 +-  0.008138
          R( 5, 3) =     1.522034 +-  0.004230
          R( 4, 2) =     1.530026 +-  0.003172
          R( 2, 1) =     1.211770 +-  0.001928
          R( 6, 4) =     1.545123 +-  0.004628
          R( 9, 6) =     1.547273 +-  0.005066
          R(11, 7) =     1.541599 +-  0.006274
          R(10, 7) =     1.533933 +-  0.005165
       A( 8, 3, 2) =   102.642355 +-  0.568250
       A( 7, 3, 2) =   100.575787 +-  0.320322
       A( 5, 3, 2) =   113.584933 +-  0.598621
       A( 3, 2, 1) =   126.797759 +-  0.119454 and at N=  4
       A( 6, 4, 2) =   101.589863 +-  0.139150
       A( 9, 6, 4) =   106.477130 +-  0.283261
```

```
       A(11, 7, 3) =   113.178305 +-  0.448844
       A(10, 7, 3) =   114.089163 +-  0.590623
    D( 4, 2, 1, 3) = [-180.000000 ]    FIXED
    D( 5, 3, 2, 1) =    16.290487 +-  0.376402
    D( 6, 4, 2, 5) =   -13.447286 +-  0.333432
    D( 7, 3, 2, 1) =   145.687415 +-  0.385646
    D( 8, 3, 2, 4) =    71.733595 +-  0.415969
    D( 9, 6, 4, 2) =   -72.331892 +-  0.188970
    D(10, 7, 3, 5) =   -62.943704 +-  0.841068
    D(11, 7, 3, 5) =    60.414052 +-  0.816670

             Chi-squared =        0.0004792367
       Deviation of fit =        0.006601
```

Ni	Axis	Iobs	Icalc	Io-c	Bobs	Bcalc	Bo-c
1	a	349.26740	349.25827	0.00913	1446.9687	1447.0066	-0.0378
1	b	427.06864	427.05737	0.01128	1183.3672	1183.3984	-0.0313
1	c	460.64947	460.63742	0.01205	1097.1010	1097.1297	-0.0287
2	a	349.81540	349.81435	0.00105	1444.7020	1444.7063	-0.0043
2	b	427.42002	427.42251	-0.00249	1182.3943	1182.3874	0.0069
2	c	460.93292	460.93467	-0.00175	1096.4264	1096.4222	0.0042
3	a	349.53692	349.53833	-0.00141	1445.8530	1445.8472	0.0058
3	b	428.11826	428.11937	-0.00111	1180.4659	1180.4629	0.0031
3	c	461.61293	461.61362	-0.00069	1094.8112	1094.8096	0.0016
4	a	349.33291	349.33268	0.00023	1446.6974	1446.6984	-0.0010
4	b	429.01885	429.02092	-0.00208	1177.9879	1177.9822	0.0057
4	c	462.55951	462.56003	-0.00052	1092.5708	1092.5696	0.0012
5	a	351.09245	351.09254	-0.00009	1439.4471	1439.4467	0.0004
5	b	427.92503	427.92594	-0.00091	1180.9990	1180.9964	0.0025
5	c	462.62203	462.62346	-0.00143	1092.4231	1092.4198	0.0034
6	a	352.28505	352.29122	-0.00617	1434.5741	1434.5490	0.0251
6	b	429.71854	429.71543	0.00312	1176.0698	1176.0783	-0.0085
6	c	461.02078	461.01911	0.00168	1096.2174	1096.2214	-0.0040
7	a	351.96995	351.96976	0.00019	1435.8584	1435.8592	-0.0008
7	b	428.70905	428.71092	-0.00187	1178.8391	1178.8340	0.0051
7	c	462.92552	462.92706	-0.00154	1091.7070	1091.7033	0.0036
8	a	352.93834	352.94076	-0.00242	1431.9187	1431.9089	0.0098
8	b	428.30476	428.30691	-0.00216	1179.9519	1179.9460	0.0059
8	c	464.28135	464.28152	-0.00017	1088.5189	1088.5185	0.0004
9	a	353.47250	353.47477	-0.00227	1429.7548	1429.7456	0.0092
9	b	430.50686	430.50814	-0.00129	1173.9163	1173.9128	0.0035
9	c	462.60958	462.61076	-0.00118	1092.4525	1092.4498	0.0028
10	a	353.97913	353.97840	0.00073	1427.7085	1427.7114	-0.0029
10	b	428.48865	428.49063	-0.00198	1179.4455	1179.4400	0.0055
10	c	464.56314	464.56537	-0.00223	1087.8586	1087.8534	0.0052
11	a	349.69389	349.69191	0.00198	1445.2040	1445.2122	-0.0082
11	b	432.44121	432.44074	0.00047	1168.6652	1168.6665	-0.0013
11	c	466.40846	466.41176	-0.00330	1083.5546	1083.5469	0.0077
12	a	349.44013	349.44103	-0.00090	1446.2535	1446.2498	0.0037
12	b	439.97008	439.97094	-0.00085	1148.6668	1148.6645	0.0022
12	c	473.53027	473.53111	-0.00085	1067.2581	1067.2562	0.0019

Correlation coefficients:

		1	2	3	4	5	6	7	8
1:	R(3, 2)	1.000							
2:	R(8, 3)	-0.363	1.000						
3:	R(7, 3)	-0.744	0.114	1.000					
4:	R(5, 3)	-0.074	-0.562	-0.146	1.000				
5:	R(4, 2)	-0.511	0.283	0.367	-0.099	1.000			
6:	R(2, 1)	0.026	-0.236	-0.083	0.200	-0.542	1.000		
7:	R(6, 4)	0.262	-0.147	-0.128	-0.009	-0.397	0.207	1.000	
8:	R(9, 6)	-0.133	0.203	0.004	-0.013	0.130	-0.029	-0.467	1.000

9:	R(11, 7)	0.084	-0.011	-0.196	-0.060	-0.044	0.005	-0.022	0.130
10:	R(10, 7)	0.005	0.080	0.192	-0.032	0.002	-0.015	0.194	-0.064
11:	A(8, 3, 2)	-0.818	-0.046	0.702	0.321	0.387	-0.074	-0.293	0.090
12:	A(7, 3, 2)	-0.521	0.310	-0.073	0.322	0.437	-0.160	-0.356	0.213
13:	A(5, 3, 2)	-0.906	0.520	0.739	-0.272	0.453	-0.108	-0.148	0.053
14:	A(3, 2, 1)	0.587	-0.367	-0.612	0.435	0.033	-0.347	-0.080	-0.029
15:	A(6, 4, 2)	0.141	-0.020	-0.146	0.027	-0.101	-0.376	-0.390	0.366
16:	A(9, 6, 4)	-0.001	-0.060	0.000	0.009	0.110	-0.060	-0.289	-0.479
17:	A(11, 7, 3)	0.266	-0.478	-0.312	0.361	-0.158	0.132	0.002	-0.178
18:	A(10, 7, 3)	-0.508	0.160	0.051	0.080	0.303	-0.052	-0.327	0.114
19:	D(5, 3, 2, 1)	-0.493	-0.412	0.622	0.252	0.294	0.004	-0.139	-0.029
20:	D(6, 4, 2, 5)	0.183	0.157	-0.240	-0.121	-0.170	0.039	-0.011	0.375
21:	D(7, 3, 2, 1)	-0.113	0.664	0.128	-0.571	0.138	-0.202	0.016	0.148
22:	D(8, 3, 2, 4)	0.720	-0.280	-0.753	0.241	-0.328	0.095	0.291	-0.214
23:	D(9, 6, 4, 2)	-0.218	0.016	0.175	0.068	0.156	-0.118	-0.214	-0.004
24:	D(10, 7, 3, 5)	-0.613	0.552	0.486	-0.257	0.333	-0.154	-0.064	0.125
25:	D(11, 7, 3, 5)	-0.771	0.443	0.315	-0.017	0.468	-0.118	-0.268	0.076

		9	10	11	12	13	14	15	16
9:	R(11, 7)	1.000							
10:	R(10, 7)	-0.571	1.000						
11:	A(8, 3, 2)	-0.091	-0.081	1.000					
12:	A(7, 3, 2)	0.212	-0.525	0.367	1.000				
13:	A(5, 3, 2)	-0.024	-0.045	0.620	0.380	1.000			
14:	A(3, 2, 1)	0.016	0.055	-0.420	0.056	-0.715	1.000		
15:	A(6, 4, 2)	0.038	-0.056	-0.077	0.106	-0.140	0.419	1.000	
16:	A(9, 6, 4)	-0.022	-0.100	0.000	0.026	0.004	0.019	-0.223	1.000
17:	A(11, 7, 3)	-0.627	0.161	-0.025	-0.111	-0.405	0.280	0.052	0.063
18:	A(10, 7, 3)	0.396	-0.762	0.474	0.769	0.498	-0.293	0.013	0.094
19:	D(5, 3, 2, 1)	-0.068	-0.059	0.688	0.022	0.355	-0.329	-0.116	0.143
20:	D(6, 4, 2, 5)	0.101	-0.029	-0.306	0.020	-0.087	0.176	0.305	-0.576
21:	D(7, 3, 2, 1)	0.501	0.021	-0.176	-0.021	0.303	-0.285	-0.083	0.046
22:	D(8, 3, 2, 4)	0.088	0.073	-0.760	-0.117	-0.729	0.705	0.059	0.147
23:	D(9, 6, 4, 2)	-0.011	-0.075	0.295	0.131	0.132	-0.141	0.134	0.456
24:	D(10, 7, 3, 5)	0.499	-0.110	0.347	0.302	0.700	-0.435	-0.095	-0.008
25:	D(11, 7, 3, 5)	0.112	-0.478	0.527	0.827	0.778	-0.408	-0.027	0.040

		17	18	19	20	21	22	23	24
17:	A(11, 7, 3)	1.000							
18:	A(10, 7, 3)	-0.105	1.000						
19:	D(5, 3, 2, 1)	0.167	0.256	1.000					
20:	D(6, 4, 2, 5)	-0.110	-0.059	-0.612	1.000				
21:	D(7, 3, 2, 1)	-0.865	-0.028	-0.284	-0.054	1.000			
22:	D(8, 3, 2, 4)	0.152	-0.407	-0.467	0.025	-0.053	1.000		
23:	D(9, 6, 4, 2)	-0.021	0.178	0.424	-0.738	0.147	-0.123	1.000	
24:	D(10, 7, 3, 5)	-0.861	0.332	0.003	0.082	0.727	-0.437	0.057	1.000
25:	D(11, 7, 3, 5)	-0.200	0.846	0.214	-0.025	0.064	-0.504	0.120	0.492

		25
25:	D(11, 7, 3, 5)	1.000

Final principal coordinates of parent:

ATOM NO.	A	B	C	MASS
1	-2.547204	0.187936	-0.213755	15.9949150
2	-1.382858	-0.147379	-0.229486	12.0000000
3	-0.230760	0.488337	0.565230	12.0000000
4	-0.768352	-1.287324	-1.044279	12.0000000
5	-0.563049	1.864528	1.124041	12.0000000
6	0.716269	-1.203805	-0.624360	12.0000000

7	0.929548	0.325749	-0.438982	12.0000000
8	0.080929	-0.594841	1.638832	12.0000000
9	0.791379	-1.728570	0.829268	12.0000000
10	2.305990	0.692768	0.129924	12.0000000
11	0.730586	1.139634	-1.733020	12.0000000
12	-1.449798	1.804649	1.756791	1.0078250
13	-0.781306	2.571791	0.321167	1.0078250
14	0.263569	2.255213	1.719313	1.0078250
15	1.413749	-1.684160	-1.316904	1.0078250
16	-0.928638	-1.106018	-2.110152	1.0078250
17	-1.245108	-2.239900	-0.799431	1.0078250
18	1.816886	-1.883799	1.170885	1.0078250
19	0.276292	-2.687598	0.915376	1.0078250
20	-0.817893	-0.939327	2.156614	1.0078250
21	0.738119	-0.159990	2.396232	1.0078250
22	3.085409	0.421803	-0.586828	1.0078250
23	2.371705	1.769892	0.297106	1.0078250
24	2.531884	0.195217	1.071909	1.0078250
25	0.890539	2.201894	-1.536852	1.0078250
26	1.455250	0.830868	-2.487875	1.0078250
27	-0.267696	1.035608	-2.160680	1.0078250

Table S4. The results of fitting the rm(1) geometry of the camphor molecule.

CAMPHOR, standard bond type declaration starting at the oxygen

---

```
!
!  CH bonds from [MP2+(1/4)(MP2-HF)]/6-31G** rounded to nearest 0.001A
!
```

NUMBER OF ATOMS = 27

NO	NA	NB	NC	NO.NA	NO.NA.NB	NO.NA.NB.NC	MASS	Fig.1
1	0	0	0	0.000000	0.000000	0.000000	15.9949150	= O
2	1	0	0	1.225510	0.000000	0.000000	12.0000000	= C2
3	2	1	0	1.527410	126.634000	0.000000	12.0000000	= C1
4	2	1	3	1.535990	126.648000	-179.703000	12.0000000	= C3
5	3	2	1	1.513010	113.903000	16.919000	12.0000000	= C10
6	4	2	5	1.537890	101.432000	-13.656000	12.0000000	= C4
7	3	2	1	1.557260	100.279000	145.912000	12.0000000	= C7
8	3	2	4	1.555860	103.308000	70.849000	12.0000000	= C6
9	6	4	2	1.542350	106.544000	-72.288000	12.0000000	= C5
10	7	3	5	1.529750	114.152000	-63.350000	12.0000000	= C9
11	7	3	5	1.532870	112.976000	60.464000	12.0000000	= C8
12	5	3	7	1.091000	109.923000	-175.885000	1.0078250	= H10
13	5	3	7	1.092000	111.058000	-57.139000	1.0078250	= H10′
14	5	3	7	1.091000	111.020000	63.929000	1.0078250	= H10′′
15	6	7	3	1.094000	114.822000	179.918000	1.0078250	= H4
16	4	2	1	1.093000	109.684000	-60.094000	1.0078250	= H3
17	4	2	1	1.093000	110.784000	58.298000	1.0078250	= H3′
18	9	8	3	1.092000	111.577000	-117.360000	1.0078250	= H5
19	9	8	3	1.092000	112.432000	122.331000	1.0078250	= H5′
20	8	9	6	1.093000	112.976000	-118.360000	1.0078250	= H8
21	8	9	6	1.093000	111.963000	120.812000	1.0078250	= H8′
22	10	7	3	1.093000	109.716000	-172.169000	1.0078250	= H9
23	10	7	3	1.092000	110.291000	69.501000	1.0078250	= H9′
24	10	7	3	1.089000	113.430000	-51.530000	1.0078250	= H9′′
25	11	7	3	1.092000	110.113000	-73.539000	1.0078250	= H8
26	11	7	3	1.091000	110.221000	167.908000	1.0078250	= H8′
27	11	7	3	1.091000	113.378000	46.667000	1.0078250	= H8′′

FINAL RESULTS OF LEAST SQUARES FIT:

```
          R( 3, 2) =     1.538489 +-  0.007292
          R( 8, 3) =     1.549294 +-  0.004469
          R( 7, 3) =     1.523952 +-  0.006902
          R( 5, 3) =     1.523716 +-  0.002624
          R( 4, 2) =     1.528235 +-  0.003073
          R( 2, 1) =     1.212981 +-  0.001225
          R( 6, 4) =     1.533033 +-  0.004701
          R( 9, 6) =     1.540865 +-  0.003940
          R(11, 7) =     1.543883 +-  0.003893
          R(10, 7) =     1.532195 +-  0.003378
       A( 8, 3, 2) =   102.321534 +-  0.414847
       A( 7, 3, 2) =   100.682451 +-  0.250123
       A( 5, 3, 2) =   113.085003 +-  0.434250
       A( 3, 2, 1) =   127.009165 +-  0.103368 and at N=  4
       A( 6, 4, 2) =   101.543784 +-  0.086088
       A( 9, 6, 4) =   106.640752 +-  0.178981
       A(11, 7, 3) =   113.115651 +-  0.287269
```

```
        A(10, 7, 3) =   114.015746 +-  0.458345
     D( 4, 2, 1, 3) = [-180.000000 ]    FIXED
     D( 5, 3, 2, 1) =    16.096812 +-  0.244086
     D( 6, 4, 2, 5) =   -13.576096 +-  0.208465
     D( 7, 3, 2, 1) =   145.750217 +-  0.244857
     D( 8, 3, 2, 4) =    72.384908 +-  0.322738
     D( 9, 6, 4, 2) =   -72.426221 +-  0.126404
     D(10, 7, 3, 5) =   -63.008871 +-  0.561715
     D(11, 7, 3, 5) =    60.013043 +-  0.602269
               c_a  =     0.086286 +-  0.026503
               c_b  =     0.133107 +-  0.029303
               c_c  =     0.119436 +-  0.027964

              Chi-squared =        0.0001284099
          Deviation of fit =        0.004006
```

Ni	Axis	Iobs	Icalc	Io-c	Bobs	Bcalc	Bo-c
1	a	349.26740	349.26319	0.00421	1446.9687	1446.9862	-0.0174
1	b	427.06864	427.06604	0.00260	1183.3672	1183.3744	-0.0072
1	c	460.64947	460.64615	0.00332	1097.1010	1097.1089	-0.0079
2	a	349.81540	349.81257	0.00283	1444.7020	1444.7137	-0.0117
2	b	427.42002	427.42117	-0.00115	1182.3943	1182.3912	0.0032
2	c	460.93292	460.93549	-0.00257	1096.4264	1096.4202	0.0061
3	a	349.53692	349.53776	-0.00083	1445.8530	1445.8496	0.0034
3	b	428.11826	428.11839	-0.00013	1180.4659	1180.4656	0.0004
3	c	461.61293	461.61195	0.00098	1094.8112	1094.8135	-0.0023
4	a	349.33291	349.33704	-0.00413	1446.6974	1446.6803	0.0171
4	b	429.01885	429.02040	-0.00155	1177.9879	1177.9836	0.0043
4	c	462.55951	462.55872	0.00079	1092.5708	1092.5727	-0.0019
5	a	351.09245	351.09216	0.00029	1439.4471	1439.4483	-0.0012
5	b	427.92503	427.92410	0.00092	1180.9990	1181.0015	-0.0025
5	c	462.62203	462.62209	-0.00006	1092.4231	1092.4230	0.0001
6	a	352.28505	352.28461	0.00044	1434.5741	1434.5759	-0.0018
6	b	429.71854	429.71881	-0.00026	1176.0698	1176.0691	0.0007
6	c	461.02078	461.02335	-0.00257	1096.2174	1096.2113	0.0061
7	a	351.96995	351.96896	0.00099	1435.8584	1435.8624	-0.0040
7	b	428.70905	428.71006	-0.00101	1178.8391	1178.8364	0.0028
7	c	462.92552	462.92548	0.00003	1091.7070	1091.7070	-0.0001
8	a	352.93834	352.93909	-0.00075	1431.9187	1431.9157	0.0030
8	b	428.30476	428.30525	-0.00049	1179.9519	1179.9506	0.0013
8	c	464.28135	464.28111	0.00025	1088.5189	1088.5194	-0.0006
9	a	353.47250	353.47479	-0.00228	1429.7548	1429.7456	0.0092
9	b	430.50686	430.50528	0.00157	1173.9163	1173.9206	-0.0043
9	c	462.60958	462.60827	0.00131	1092.4525	1092.4556	-0.0031
10	a	353.97913	353.97637	0.00276	1427.7085	1427.7196	-0.0111
10	b	428.48865	428.48866	-0.00001	1179.4455	1179.4455	0.0000
10	c	464.56314	464.56528	-0.00213	1087.8586	1087.8536	0.0050
11	a	349.69389	349.69285	0.00104	1445.2040	1445.2083	-0.0043
11	b	432.44121	432.44163	-0.00042	1168.6652	1168.6641	0.0011
11	c	466.40846	466.40762	0.00083	1083.5546	1083.5565	-0.0019
12	a	349.44013	349.44470	-0.00457	1446.2535	1446.2346	0.0189
12	b	439.97008	439.97015	-0.00006	1148.6668	1148.6666	0.0002
12	c	473.53027	473.53046	-0.00019	1067.2581	1067.2577	0.0004

Correlation coefficients:

		1	2	3	4	5	6	7	8
1:	R(3, 2)	1.000							
2:	R(8, 3)	-0.350	1.000						
3:	R(7, 3)	-0.639	0.317	1.000					
4:	R(5, 3)	0.039	-0.582	-0.252	1.000				
5:	R(4, 2)	0.021	0.185	0.146	-0.048	1.000			
6:	R(2, 1)	0.129	-0.311	-0.252	0.244	-0.281	1.000		

```
 7:          R( 6, 4)  -0.167  0.190  0.395 -0.140 -0.497 -0.081  1.000
 8:          R( 9, 6)   0.078  0.107  0.165 -0.028  0.328 -0.029 -0.248  1.000
 9:          R(11, 7)   0.087 -0.034 -0.226 -0.045 -0.022  0.035 -0.089  0.003
10:          R(10, 7)   0.169  0.068  0.133 -0.009  0.261  0.008 -0.021  0.142
11:       A( 8, 3, 2)  -0.855  0.048  0.676  0.156 -0.098 -0.186  0.215 -0.021
12:       A( 7, 3, 2)  -0.651  0.294  0.044  0.181 -0.168 -0.198  0.110 -0.180
13:       A( 5, 3, 2)  -0.906  0.531  0.757 -0.346  0.057 -0.229  0.282 -0.006
14:       A( 3, 2, 1)   0.656 -0.454 -0.723  0.449  0.315 -0.044 -0.590  0.030
15:       A( 6, 4, 2)   0.117  0.013 -0.014  0.021  0.012 -0.378 -0.206  0.382
16:       A( 9, 6, 4)   0.074 -0.096 -0.163  0.054  0.146 -0.005 -0.347 -0.419
17:       A(11, 7, 3)   0.309 -0.461 -0.238  0.374 -0.028  0.151 -0.064  0.021
18:       A(10, 7, 3)  -0.661  0.200  0.202 -0.026 -0.244 -0.145  0.202 -0.157
19:    D( 5, 3, 2, 1)  -0.527 -0.300  0.613  0.169  0.069 -0.077  0.122  0.037
20:    D( 6, 4, 2, 5)   0.226  0.179 -0.119 -0.125  0.054  0.035 -0.043  0.395
21:    D( 7, 3, 2, 1)  -0.198  0.602  0.107 -0.565 -0.061 -0.211  0.116 -0.045
22:    D( 8, 3, 2, 4)   0.722 -0.443 -0.819  0.339 -0.035  0.255 -0.307 -0.112
23:    D( 9, 6, 4, 2)  -0.096 -0.062  0.200  0.062  0.168 -0.106 -0.119  0.236
24:    D(10, 7, 3, 5)  -0.670  0.535  0.449 -0.307  0.037 -0.213  0.155 -0.066
25:    D(11, 7, 3, 5)  -0.837  0.448  0.435 -0.121 -0.031 -0.219  0.217 -0.082
26:             c_a    -0.277 -0.216 -0.312  0.062 -0.632  0.072  0.011 -0.471
27:             c_b     0.114 -0.343 -0.648  0.167 -0.056  0.239 -0.602 -0.345
28:             c_c     0.149 -0.459 -0.616  0.183 -0.096  0.256 -0.597 -0.158

                           9     10     11     12     13     14     15     16

 9:          R(11, 7)   1.000
10:          R(10, 7)  -0.538  1.000
11:       A( 8, 3, 2)  -0.122 -0.205  1.000
12:       A( 7, 3, 2)   0.179 -0.601  0.506  1.000
13:       A( 5, 3, 2)  -0.063 -0.139  0.715  0.482  1.000
14:       A( 3, 2, 1)   0.077  0.166 -0.598 -0.253 -0.777  1.000
15:       A( 6, 4, 2)   0.009 -0.003 -0.046  0.032 -0.081  0.261  1.000
16:       A( 9, 6, 4)   0.040 -0.086 -0.108 -0.007 -0.105  0.176 -0.233  1.000
17:       A(11, 7, 3)  -0.624  0.213 -0.082 -0.215 -0.398  0.266  0.072  0.033
18:       A(10, 7, 3)   0.296 -0.764  0.623  0.843  0.605 -0.511 -0.019  0.002
19:    D( 5, 3, 2, 1)  -0.109 -0.095  0.711  0.108  0.446 -0.413 -0.069  0.037
20:    D( 6, 4, 2, 5)   0.082  0.058 -0.319 -0.104 -0.097  0.153  0.319 -0.536
21:    D( 7, 3, 2, 1)   0.499 -0.072 -0.055  0.135  0.320 -0.297 -0.108  0.050
22:    D( 8, 3, 2, 4)   0.121  0.120 -0.765 -0.280 -0.794  0.807  0.003  0.234
23:    D( 9, 6, 4, 2)  -0.071  0.017  0.219 -0.060  0.087 -0.070  0.184  0.347
24:    D(10, 7, 3, 5)   0.463 -0.211  0.438  0.438  0.722 -0.484 -0.091 -0.027
25:    D(11, 7, 3, 5)   0.065 -0.520  0.661  0.837  0.833 -0.588 -0.016 -0.054
26:             c_a     0.076 -0.331  0.208  0.445  0.053 -0.043 -0.137  0.042
27:             c_b     0.143 -0.091 -0.238  0.039 -0.319  0.503 -0.133  0.218
28:             c_c     0.087 -0.062 -0.213 -0.059 -0.331  0.514 -0.095  0.166

                           17     18     19     20     21     22     23     24

17:       A(11, 7, 3)   1.000
18:       A(10, 7, 3)  -0.191  1.000
19:    D( 5, 3, 2, 1)   0.149  0.327  1.000
20:    D( 6, 4, 2, 5)  -0.078 -0.152 -0.569  1.000
21:    D( 7, 3, 2, 1)  -0.868  0.118 -0.246 -0.088  1.000
22:    D( 8, 3, 2, 4)   0.200 -0.505 -0.501  0.019 -0.126  1.000
23:    D( 9, 6, 4, 2)   0.086  0.032  0.419 -0.611  0.034 -0.062  1.000
24:    D(10, 7, 3, 5)  -0.855  0.461  0.075  0.031  0.734 -0.500 -0.043  1.000
25:    D(11, 7, 3, 5)  -0.255  0.880  0.321 -0.085  0.159 -0.616  0.037  0.583
26:             c_a    -0.108  0.382  0.008 -0.225  0.171  0.102 -0.184  0.156
27:             c_b    -0.039 -0.097 -0.221 -0.110  0.032  0.474 -0.182 -0.066
28:             c_c     0.061 -0.138 -0.159 -0.102 -0.039  0.529 -0.020 -0.145

                           25     26     27     28

25:    D(11, 7, 3, 5)   1.000
26:             c_a     0.208  1.000
```

```
27:              c_b   -0.210  0.619  1.000
28:              c_c   -0.238  0.600  0.907  1.000
```

Final principal coordinates of parent:

ATOM NO.	A	B	C	MASS
1	-2.542571	0.189882	-0.209605	15.9949150
2	-1.377342	-0.146566	-0.228757	12.0000000
3	-0.217778	0.485703	0.560289	12.0000000
4	-0.761787	-1.284937	-1.041595	12.0000000
5	-0.556379	1.861807	1.120107	12.0000000
6	0.710039	-1.201256	-0.620983	12.0000000
7	0.924273	0.320914	-0.435198	12.0000000
8	0.076921	-0.591000	1.634614	12.0000000
9	0.785963	-1.725589	0.825936	12.0000000
10	2.300615	0.689672	0.128116	12.0000000
11	0.722804	1.138120	-1.729477	12.0000000
12	-1.440939	1.797327	1.755463	1.0078250
13	-0.780861	2.567510	0.317576	1.0078250
14	0.269806	2.257292	1.712804	1.0078250
15	1.405112	-1.681406	-1.316083	1.0078250
16	-0.923289	-1.105359	-2.107578	1.0078250
17	-1.236337	-2.238199	-0.795134	1.0078250
18	1.808802	-1.886880	1.172708	1.0078250
19	0.265672	-2.682290	0.906471	1.0078250
20	-0.822188	-0.934279	2.152700	1.0078250
21	0.734612	-0.156319	2.391677	1.0078250
22	3.078175	0.416096	-0.589662	1.0078250
23	2.366709	1.767408	0.291149	1.0078250
24	2.528992	0.195612	1.071339	1.0078250
25	0.887487	2.199571	-1.532839	1.0078250
26	1.443262	0.827478	-2.487582	1.0078250
27	-0.277576	1.038249	-2.153205	1.0078250

Terms in I.fitted = I.rigid + eps

Ni	(I_a)rig	(I_b)rig	(I_c)rig	eps_a	eps_b	eps_c
1	347.65435	424.32414	458.08985	1.60884	2.74191	2.55630
2	348.20245	424.67815	458.37841	1.61012	2.74302	2.55709
3	347.92825	425.37308	459.05295	1.60950	2.74531	2.55900
4	347.72801	426.27224	459.99716	1.60903	2.74815	2.56156
5	349.47891	425.17972	460.06026	1.61325	2.74438	2.56182
6	350.66881	426.96844	458.46591	1.61580	2.75036	2.55744
7	350.35358	425.96324	460.36277	1.61538	2.74682	2.56272
8	351.32138	425.55993	461.71461	1.61771	2.74531	2.56649
9	351.85590	427.75285	460.04633	1.61889	2.75244	2.56194
10	352.35644	425.74266	461.99789	1.61993	2.74601	2.56739
11	348.08253	429.68296	463.83537	1.61032	2.75867	2.57226
12	347.83510	437.18720	470.93872	1.60960	2.78295	2.59174

Table S5. The observed and the obs.-calc. frequencies (MHz) of measured Stark components of rotational transitions in the parent isopomer of camphor.

TRANSITIONS (F and MF in units of 1/2):

	J	K -1	K +1	<- J	K -1	K +1	F	MF	<- F	MF	Volts	Obs	Obs-Calc
1.	4	2	3	3	1	2	8	0	6	0	0.0	9781.80900	0.00017
2.	4	2	3	3	1	2	8	2	6	2	945.7	9781.65700	-0.00206
3.	4	2	3	3	1	2	8	2	6	2	1336.4	9781.50850	-0.00135
4.	4	2	3	3	1	2	8	2	6	2	1636.5	9781.36230	0.00165
5.	4	2	3	3	1	2	8	2	6	2	1888.4	9781.21250	0.00023
6.	4	2	3	3	1	2	8	2	6	2	2113.5	9781.06010	-0.00173
7.	5	3	3	4	2	2	10	2	8	2	0.0	12799.97630	-0.00002
8.	5	3	3	4	2	2	10	2	8	2	568.5	12799.78300	-0.00091
9.	5	3	3	4	2	2	10	2	8	2	798.8	12799.60060	0.00344
10.	5	3	3	4	2	2	10	2	8	2	982.2	12799.40570	0.00150
11.	5	2	4	4	1	3	10	0	8	0	0.0	11893.77040	-0.00053
12.	5	2	4	4	1	3	10	2	8	2	2529.7	11893.54610	-0.00424
13.	5	2	4	4	1	3	10	2	8	2	3581.8	11893.32750	-0.00134
14.	5	2	4	4	1	3	10	2	8	2	4370.9	11893.11020	-0.00260
15.	5	2	4	4	1	3	10	2	8	2	5057.8	11892.88760	-0.00239
16.	5	2	4	4	1	3	10	2	8	2	5668.5	11892.66160	-0.00318
17.	5	2	4	4	1	3	10	2	8	2	6196.2	11892.44880	-0.00087
18.	5	2	4	4	1	3	10	4	8	4	1131.0	11893.61740	-0.00299
19.	5	2	4	4	1	3	10	4	8	4	1603.9	11893.46570	-0.00257
20.	5	2	4	4	1	3	10	4	8	4	1965.8	11893.31510	-0.00131
21.	5	2	4	4	1	3	10	4	8	4	2267.4	11893.16170	-0.00473
22.	5	2	4	4	1	3	10	4	8	4	2535.6	11893.01350	-0.00170
23.	5	2	4	4	1	3	10	4	8	4	2778.8	11892.86150	-0.00205
24.	5	2	4	4	1	3	10	4	8	4	2998.9	11892.71130	-0.00314
25.	4	0	4	3	0	3	8	0	6	0	0.0	8975.68320	-0.00010
26.	4	0	4	3	0	3	8	4	6	4	2530.5	8975.89860	0.00161
27.	4	0	4	3	0	3	8	4	6	4	3582.4	8976.11580	0.00221
28.	4	0	4	3	0	3	8	4	6	4	4371.6	8976.32710	0.00007
29.	4	0	4	3	0	3	8	4	6	4	5060.7	8976.55080	0.00068
30.	4	0	4	3	0	3	8	4	6	4	6203.3	8976.99990	0.00168
31.	4	0	4	3	0	3	8	4	6	4	7161.4	8977.45420	0.00162
32.	4	0	4	3	0	3	8	4	6	4	8000.4	8977.91100	-0.00159
33.	4	0	4	3	0	3	8	6	6	6	2530.5	8976.26330	0.00010
34.	4	0	4	3	0	3	8	6	6	6	3582.4	8976.85790	0.00290
35.	4	0	4	3	0	3	8	6	6	6	4371.6	8977.44040	-0.00172
36.	4	0	4	3	0	3	8	6	6	6	5060.7	8978.06580	0.00574
37.	4	1	3	3	1	2	8	0	6	0	0.0	9250.65450	-0.00174
38.	4	1	3	3	1	2	8	2	6	2	2530.5	9250.40160	-0.00070
39.	4	1	3	3	1	2	8	2	6	2	3577.0	9250.15100	0.00185
40.	4	1	3	3	1	2	8	4	6	4	2530.5	9249.77780	0.00104
41.	4	1	3	3	1	2	8	4	6	4	3577.0	9248.90720	0.00223

```
 42.   4  1  3   3  1  2    8  4   6  4    4383.1     9248.04230      0.00653
!-------------------------------------------------------------------------------
 43.   5  2  4   4  2  3   10  0   8  0       0.0    11362.61760     -0.00073

 44.   5  2  4   4  2  3   10  2   8  2    2530.1    11363.21460      0.00107
 45.   5  2  4   4  2  3   10  2   8  2    3577.0    11363.79900     -0.00419
 46.   5  2  4   4  2  3   10  2   8  2    4383.1    11364.38730     -0.00295
 47.   5  2  4   4  2  3   10  2   8  2    5061.5    11364.96630     -0.00551
 48.   5  2  4   4  2  3   10  2   8  2    5660.9    11365.55380      0.00321
!-------------------------------------------------------------------------------
 49.   5  1  4   4  1  3   10  0   8  0       0.0    11514.45900     -0.00101

 50.   5  1  4   4  1  3   10  4   8  4    2527.3    11514.29930     -0.00267
 51.   5  1  4   4  1  3   10  4   8  4    3583.8    11514.14040     -0.00226
 52.   5  1  4   4  1  3   10  4   8  4    4381.0    11513.98550     -0.00090
 53.   5  1  4   4  1  3   10  4   8  4    5064.9    11513.82640     -0.00145
 54.   5  1  4   4  1  3   10  4   8  4    5664.7    11513.66990     -0.00044
 55.   5  1  4   4  1  3   10  4   8  4    6200.5    11513.51440     -0.00077
 56.   5  1  4   4  1  3   10  4   8  4    6702.0    11513.35680     -0.00088

 57.   5  1  4   4  1  3   10  6   8  6    2527.3    11514.13690     -0.00176
 58.   5  1  4   4  1  3   10  6   8  6    3583.8    11513.81600     -0.00002
 59.   5  1  4   4  1  3   10  6   8  6    4381.0    11513.49860     -0.00228
 60.   5  1  4   4  1  3   10  6   8  6    5064.9    11513.18110     -0.00137
 61.   5  1  4   4  1  3   10  6   8  6    5664.7    11512.86790      0.00040
 62.   5  1  4   4  1  3   10  6   8  6    6200.5    11512.55660     -0.00197
 63.   5  1  4   4  1  3   10  6   8  6    6702.0    11512.24480     -0.00162
!-------------------------------------------------------------------------------
 64.   5  2  3   4  2  2   10  0   8  0       0.0    11599.93810     -0.00137

 65.   5  2  3   4  2  2   10  2   8  2    2527.3    11599.33430      0.00124
 66.   5  2  3   4  2  2   10  2   8  2    3583.8    11598.72610      0.00118
 67.   5  2  3   4  2  2   10  2   8  2    4381.0    11598.13260      0.00110
 68.   5  2  3   4  2  2   10  2   8  2    5064.9    11597.53420      0.00180
 69.   5  2  3   4  2  2   10  2   8  2    5664.7    11596.94620      0.00606
!-------------------------------------------------------------------------------
 70.   6  1  5   5  1  4   12  0  10  0       0.0    13741.90280     -0.00013

 71.   6  1  5   5  1  4   12  4  10  4    3577.9    13741.83400     -0.00366
 72.   6  1  5   5  1  4   12  4  10  4    5059.8    13741.76980     -0.00295
 73.   6  1  5   5  1  4   12  4  10  4    6199.9    13741.70480     -0.00320
 74.   6  1  5   5  1  4   12  4  10  4    9643.3    13741.43780      0.00100
 75.   6  1  5   5  1  4   12  4  10  4   10403.5    13741.36060     -0.00161

 76.   6  1  5   5  1  4   12  6  10  6    3577.9    13741.79390     -0.00416
 77.   6  1  5   5  1  4   12  6  10  6    5059.8    13741.69230     -0.00262
 78.   6  1  5   5  1  4   12  6  10  6    6199.9    13741.59060     -0.00262
 79.   6  1  5   5  1  4   12  6  10  6    8454.3    13741.33960     -0.00005
 80.   6  1  5   5  1  4   12  6  10  6    9640.2    13741.17840     -0.00294
 81.   6  1  5   5  1  4   12  6  10  6   10403.5    13741.07180      0.00020

 82.   6  1  5   5  1  4   12  8  10  8    5059.8    13741.58820     -0.00128
 83.   6  1  5   5  1  4   12  8  10  8    6199.9    13741.43800     -0.00254
 84.   6  1  5   5  1  4   12  8  10  8    8455.7    13741.07920     -0.00389
 85.   6  1  5   5  1  4   12  8  10  8    9643.7    13740.87300      0.00161
 86.   6  1  5   5  1  4   12  8  10  8   10403.6    13740.73340      0.00179

 87.   6  1  5   5  1  4   12 10  10 10    8454.3    13740.80200     -0.00229
 88.   6  1  5   5  1  4   12 10  10 10    9643.3    13740.56210      0.00060
 89.   6  1  5   5  1  4   12 10  10 10   10403.6    13740.41700      0.00109
!-------------------------------------------------------------------------------
 90.   6  2  4   5  2  3   12  0  10  0       0.0    13929.05040      0.00315

 91.   6  2  4   5  2  3   12  2  10  2    2530.2    13928.92160     -0.00265
 92.   6  2  4   5  2  3   12  2  10  2    3577.9    13928.80020     -0.00119
```

```
 93.   6  2  4   5  2  3   12  2  10  2    4379.7    13928.67860     -0.00040
 94.   6  2  4   5  2  3   12  2  10  2    5059.8    13928.55620      0.00026
 95.   6  2  4   5  2  3   12  2  10  2    5661.4    13928.43240     -0.00001
 96.   6  2  4   5  2  3   12  2  10  2    6199.9    13928.31150      0.00133
 97.   6  2  4   5  2  3   12  4  10  4    5661.4    13926.72850      0.00272
!
!-------------------------------------------------------------------------------
!
! Transitions affected by closest mu_c-type near-degeneracies
!
 98.   5  0  5   4  0  4   10  0   8  0       0.0    11162.93550      0.00015

 99.   5  0  5   4  0  4   10  4   8  4    2529.5    11162.99420      0.00243
100.   5  0  5   4  0  4   10  4   8  4    3577.0    11163.05380      0.00532
101.   5  0  5   4  0  4   10  4   8  4    4383.1    11163.11160      0.00590
102.   5  0  5   4  0  4   10  4   8  4    5061.5    11163.15980     -0.00335
103.   5  0  5   4  0  4   10  4   8  4    5662.6    11163.21830     -0.00297

104.   5  0  5   4  0  4   10  6   8  6    2529.5    11163.11340      0.00520
!-------------------------------------------------------------------------------
105.   5  1  5   4  1  4   10  0   8  0       0.0    11128.70380     -0.00005

106.   5  1  5   4  1  4   10  4   8  4    2531.2    11128.91200      0.00321
107.   5  1  5   4  1  4   10  4   8  4    3580.5    11129.11770      0.00417
108.   5  1  5   4  1  4   10  4   8  4    4378.7    11129.31980      0.00383
109.   5  1  5   4  1  4   10  4   8  4    5061.5    11129.52450      0.00352
110.   5  1  5   4  1  4   10  4   8  4    5662.6    11129.72470     -0.00091

 Standard deviation =       0.002562


 ITERATION NO = 5 CONSTANTS, deviations and changes:

     Mu.a     =         2.993369735 +-      0.000358852          0.000000000
     Mu.b     =        -0.729836250 +-      0.000242931          0.000000000
     Mu.c     =        -0.080441770 +-      0.000674137          0.000000000


 FINAL RESULTS OF LEAST SQUARES FITTING PROCEDURE
 ================================================

 FITTED CONSTANTS:

 A     /MHz        1446.968977          1:Xab /MHz           0.
 B     /MHz        1183.367110          1:XJ.a/kHz           0.
 C     /MHz        1097.101031          1:XK.a/kHz           0.
 DJ    /kHz           0.03348038        1:XJbc/kHz           0.
 DJK   /kHz           0.08368131        1:Ma  /MHz           0.
 DK    /kHz          -0.06557013        1:Mb-c/MHz           0.
 dJ    /kHz           0.0028638         1:Tr  /MHz           0.
 dK    /kHz           0.02485841        1:Xd  /kHz           0.
 HJ    / Hz           0.
 HJK   / Hz           0.
 HKJ   / Hz           0.
 HK    / Hz           0.
 hJ    / Hz           0.
 hJK   / Hz           0.                Mu.a  /D             2.99336(35)
 hK    / Hz           0.                Mu.b  /D            -0.72983(24)
 LKKJ  /mHz           0.                Mu.c  /D            -0.08044(67)
 1:Xa  /MHz           0.                 d    /cm           26.93
 1:Xb-c/MHz           0.                 k    /cm            0.


 CORRELATION COEFFICIENTS:
```

	Mu.a	Mu.b	Mu.c
Mu.a	1.0000		
Mu.b	-0.3513	1.0000	
Mu.c	0.0259	-0.6773	1.0000
