Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Identification of the maze in the conformational landscape of fenchol

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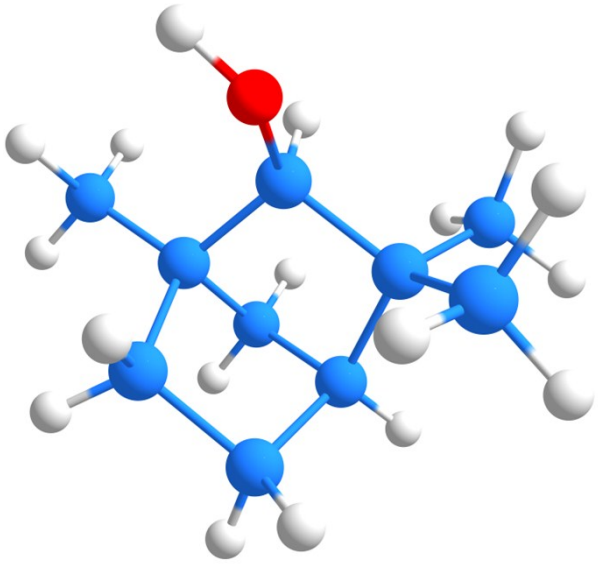
Structure of 1EF conformer

Standard orientation:

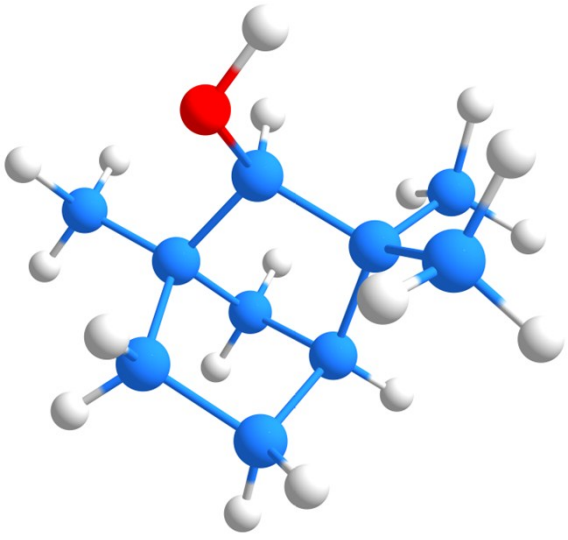
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.247224	-0.090620	0.216460
2	6	0	-1.285365	0.749011	-1.080297
3	6	0	-0.160235	1.803156	-0.876393
4	6	0	0.522352	1.315757	0.413004
5	6	0	-0.717873	0.928013	1.241057
6	6	0	1.207566	-0.060495	0.178434
7	6	0	-0.022200	-1.025185	0.151146
8	6	0	2.037241	-0.119891	-1.106741
9	6	0	2.124760	-0.402208	1.358641
10	6	0	-2.547070	-0.802388	0.544722
11	8	0	0.022412	-1.884719	-0.984953
12	1	0	1.199527	2.050814	0.863018
13	1	0	-0.489395	0.472651	2.211500
14	1	0	-1.406199	1.768218	1.395125
15	1	0	-0.015195	-1.641393	1.065897
16	1	0	1.423726	-0.050677	-2.006911
17	1	0	2.765097	0.700862	-1.110065
18	1	0	2.584522	-1.066274	-1.158717
19	1	0	2.473222	-1.438941	1.279143
20	1	0	3.003285	0.254069	1.362707
21	1	0	1.610596	-0.289324	2.319076
22	1	0	-2.831620	-1.495773	-0.257502
23	1	0	-3.366364	-0.083674	0.659073
24	1	0	-2.458935	-1.373512	1.477259
25	1	0	-0.691038	-2.522303	-0.878732
26	1	0	-1.116834	0.117756	-1.958313
27	1	0	-2.266516	1.225359	-1.190710
28	1	0	0.519281	1.881467	-1.727859
29	1	0	-0.588172	2.797537	-0.704567



Structure of 2EF conformer

Standard orientation:

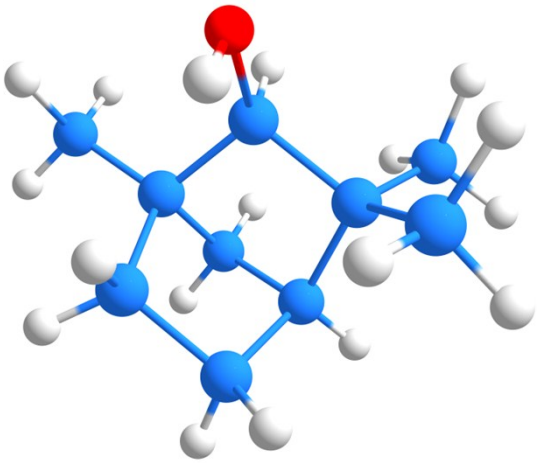
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.021998	-1.026308	0.142344
2	6	0	-1.245081	-0.101629	0.229035
3	6	0	-1.311243	0.726773	-1.075607
4	6	0	-0.173971	1.775822	-0.911965
5	6	0	0.517694	1.323390	0.386425
6	6	0	-0.714331	0.940846	1.228207
7	6	0	1.211882	-0.051414	0.182846
8	6	0	-2.530860	-0.825788	0.581775
9	6	0	2.066993	-0.124381	-1.083522
10	6	0	2.104240	-0.373839	1.387481
11	8	0	-0.132355	-1.852988	-1.013271
12	1	0	-1.181368	0.090234	-1.954990
13	1	0	-2.291251	1.211770	-1.152430
14	1	0	0.499526	1.822386	-1.770897
15	1	0	-0.589273	2.779789	-0.767649
16	1	0	1.190600	2.074761	0.816355
17	1	0	-0.479066	0.510209	2.207864
18	1	0	-1.410174	1.777580	1.365547
19	1	0	-0.006775	-1.665886	1.040410
20	1	0	-2.782279	-1.557459	-0.193484
21	1	0	-3.362400	-0.117256	0.670734
22	1	0	-2.429514	-1.358992	1.534894
23	1	0	1.467424	-0.086876	-1.994982
24	1	0	2.784942	0.704556	-1.096433
25	1	0	2.643052	-1.058041	-1.104654
26	1	0	2.473993	-1.405447	1.326131
27	1	0	2.972875	0.295136	1.411975
28	1	0	1.565732	-0.267379	2.334631
29	1	0	0.572840	-2.506014	-0.968970



Structure of 3EF conformer

Standard orientation:

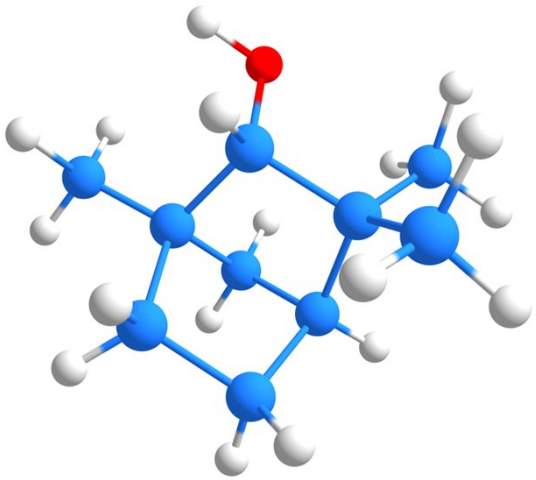
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.249165	-0.108842	0.213272
2	6	0	-1.298495	0.770672	-1.058487
3	6	0	-0.176149	1.824981	-0.836295
4	6	0	0.512651	1.311400	0.439888
5	6	0	-0.726470	0.895005	1.256012
6	6	0	1.208453	-0.053649	0.177211
7	6	0	-0.018609	-1.035708	0.137125
8	6	0	2.032671	-0.084597	-1.111486
9	6	0	2.135871	-0.412198	1.343466
10	6	0	-2.539704	-0.842051	0.525045
11	8	0	-0.029068	-1.988213	-0.915532
12	1	0	-1.156937	0.185383	-1.976342
13	1	0	-2.283350	1.243417	-1.145006
14	1	0	0.498063	1.932377	-1.689209
15	1	0	-0.611628	2.811117	-0.639481
16	1	0	1.180863	2.044103	0.906938
17	1	0	-0.496930	0.418895	2.215844
18	1	0	-1.419912	1.727420	1.428149
19	1	0	1.430217	0.058067	-2.014526
20	1	0	2.785055	0.712863	-1.091734
21	1	0	2.550576	-1.044270	-1.206198
22	1	0	2.492036	-1.444214	1.240702
23	1	0	3.008549	0.251928	1.362547
24	1	0	1.621696	-0.326509	2.306535
25	1	0	-2.775751	-1.560770	-0.267363
26	1	0	-3.376227	-0.139383	0.615185
27	1	0	-2.452138	-1.396807	1.466731
28	1	0	-0.011349	-1.654054	1.044019
29	1	0	-0.036616	-1.503937	-1.747036



Structure of 1XF conformer

Standard orientation:

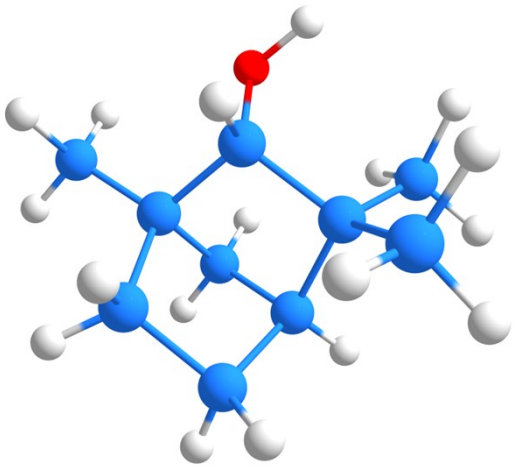
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.246462	-0.088096	-0.029370
2	6	0	-1.287109	1.318099	-0.675484
3	6	0	-0.169388	2.107055	0.062226
4	6	0	0.512538	1.005788	0.889547
5	6	0	-0.719410	0.226855	1.382050
6	6	0	1.202057	-0.035741	-0.039355
7	6	0	-0.021546	-0.812672	-0.628912
8	6	0	2.121984	-0.933972	0.797939
9	6	0	2.039680	0.592345	-1.157482
10	6	0	-2.553442	-0.852611	-0.139949
11	8	0	0.051825	-2.187008	-0.242139
12	1	0	-0.479157	-0.679861	1.945445
13	1	0	-1.410770	0.847849	1.965527
14	1	0	-0.033703	-0.746971	-1.728560
15	1	0	2.790685	1.276331	-0.743564
16	1	0	2.565814	-0.194001	-1.711319
17	1	0	1.426452	1.149276	-1.872599
18	1	0	1.606348	-1.367063	1.658309
19	1	0	2.962249	-0.330821	1.162177
20	1	0	2.518521	-1.757837	0.198423
21	1	0	-3.373131	-0.269967	0.295004
22	1	0	-2.503913	-1.808224	0.392650
23	1	0	-2.807074	-1.049002	-1.190475
24	1	0	-0.654233	-2.645091	-0.709167
25	1	0	-1.118986	1.261651	-1.758546
26	1	0	-2.271122	1.775502	-0.520946
27	1	0	-0.606062	2.851424	0.737671
28	1	0	0.508766	2.635781	-0.612057
29	1	0	1.191309	1.384791	1.661870



Structure of 2XF conformer

Standard orientation:

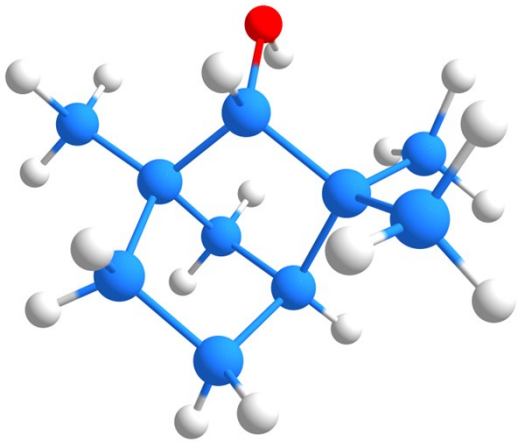
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.246473	-0.100728	-0.042321
2	6	0	-1.284395	1.316422	-0.665819
3	6	0	-0.182753	2.103015	0.097284
4	6	0	0.501837	0.991572	0.908144
5	6	0	-0.728850	0.196801	1.378636
6	6	0	1.200982	-0.024090	-0.042832
7	6	0	-0.022446	-0.819093	-0.633370
8	6	0	2.142978	-0.916525	0.773301
9	6	0	2.014806	0.635403	-1.160587
10	6	0	-2.550379	-0.866426	-0.177141
11	8	0	-0.089439	-2.187062	-0.226452
12	1	0	-0.492886	-0.717533	1.931169
13	1	0	-1.427928	0.806839	1.964016
14	1	0	1.174854	1.361000	1.690633
15	1	0	0.495530	2.653784	-0.559138
16	1	0	-0.632651	2.827831	0.785111
17	1	0	-1.104710	1.278351	-1.747508
18	1	0	-2.274250	1.761720	-0.515110
19	1	0	-0.029513	-0.767210	-1.733754
20	1	0	2.963297	-0.305200	1.166659
21	1	0	2.594896	-1.700542	0.152519
22	1	0	1.634023	-1.398650	1.611295
23	1	0	2.558980	-0.128863	-1.729116
24	1	0	2.751353	1.335875	-0.748267
25	1	0	1.381026	1.181305	-1.865731
26	1	0	-2.803224	-1.015711	-1.234106
27	1	0	-2.481242	-1.848643	0.296395
28	1	0	-3.366164	-0.302716	0.290381
29	1	0	0.702281	-2.623246	-0.555585



Structure of 3XF conformer

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.248304	-0.106791	-0.031797
2	6	0	-1.303517	1.304701	-0.668166
3	6	0	-0.191720	2.104665	0.065967
4	6	0	0.501105	1.009808	0.892003
5	6	0	-0.726865	0.220940	1.381041
6	6	0	1.201554	-0.021443	-0.039443
7	6	0	-0.017535	-0.816523	-0.638368
8	6	0	2.037558	0.613830	-1.153878
9	6	0	2.128826	-0.912015	0.797449
10	6	0	-2.549238	-0.878905	-0.152768
11	8	0	0.009864	-2.220693	-0.395610
12	1	0	-1.142393	1.253515	-1.752058
13	1	0	-2.291922	1.749234	-0.504797
14	1	0	-0.631998	2.846879	0.741300
15	1	0	0.482236	2.637003	-0.609489
16	1	0	1.173645	1.394806	1.667305
17	1	0	-0.483238	-0.670504	1.972146
18	1	0	-1.427595	0.835671	1.959315
19	1	0	2.779614	1.308616	-0.741266
20	1	0	2.573072	-0.167550	-1.705694
21	1	0	1.418180	1.160020	-1.871726
22	1	0	1.634811	-1.314851	1.688961
23	1	0	2.980774	-0.314891	1.142144
24	1	0	2.509514	-1.751135	0.208294
25	1	0	-3.365035	-0.321328	0.321896
26	1	0	-2.479790	-1.863586	0.317841
27	1	0	-2.808885	-1.032740	-1.206998
28	1	0	0.041366	-2.351232	0.557535
29	1	0	-0.032442	-0.741985	-1.732069



ENDO-Fenchol 2EF

							obs	o-c	error	blends o-c	blends wt	Notes
/ instead of : below denotes (o-c)>3*err												
1:	3	1	3	2	1	2	6061.1578	-0.0002	0.001			
2:	3	0	3	2	0	2	6167.0283	-0.0009	0.001			
3:	3	1	2	2	0	2	7070.0778	-0.0009	0.001			
4:	4	1	4	3	1	3	8062.8098	-0.0004	0.001			
5:	4	0	4	3	0	3	8153.1275	-0.0004	0.001			
6:	4	2	3	3	2	2	8308.6127	-0.0003	0.001			
7:	4	2	2	3	2	1	8479.5559	-0.0002	0.001			
8:	4	1	3	3	1	2	8504.3063	-0.0005	0.001			
9:	3	3	0	2	2	0	8635.4690	-0.0002	0.001			
10:	3	3	1	2	2	1	8653.2209	-0.0002	0.001			
11:	3	1	2	2	1	1	6399.9050	0.0000	0.001			
12:	3	2	1	2	1	1	7607.9645	0.0021	0.001			
13:	3	2	2	2	1	2	7852.7745	-0.0005	0.001			
14:	4	1	3	3	2	1	7296.2537	0.0042	0.003			
15:	4	0	4	3	1	2	7250.0758	-0.0027	0.001			
16:	3	2	1	2	2	0	6319.4021	0.0055	0.003			
17:	3	2	2	2	2	1	6243.2115	-0.0017	0.001			
18:	2	2	1	1	1	1	5658.0446	0.0013	0.001			
19:	2	2	0	1	1	0	5564.3725	0.0009	0.001			
20:	3	0	3	2	1	1	5496.8547	-0.0008	0.001			
21:	2	1	1	1	0	1	4812.3238	-0.0027	0.001			
22:	2	0	2	1	0	1	4142.1530	0.0002	0.001			
23:	2	1	2	1	1	1	4048.4810	-0.0004	0.001			
24:	1	1	0	0	0	0	2617.5920	-0.0010	0.001			
25:	4	3	2	3	3	1	8358.4266	0.0007	0.001			
26:	5	1	4	4	2	2	9394.7186	0.0001	0.001			
27:	4	1	3	3	0	3	9407.3576	0.0012	0.001			
28:	4	2	2	3	1	2	9687.6128	-0.0007	0.001			
29:	6	1	6	5	2	4	9690.8126	0.0020	0.001			
30:	6	2	5	5	3	3	9845.6865	0.0028	0.001			
31:	5	1	5	4	1	4	10053.6595	0.0001	0.001			
32:	5	0	5	4	0	4	10115.3041	-0.0002	0.001			
33:	4	2	3	3	1	3	10100.2300	0.0000	0.001			
34:	5	2	4	4	2	3	10361.0406	-0.0001	0.001			
35:	5	4	2	4	4	1	10449.6462	0.0008	0.001			
36:	5	4	1	4	4	0	10451.2829	0.0012	0.001			
37:	5	3	3	4	3	2	10453.8758	-0.0002	0.001			
38:	5	3	2	4	3	1	10497.7980	-0.0004	0.001			
39:	5	1	4	4	1	3	10578.0250	-0.0001	0.001			
40:	5	2	3	4	2	2	10649.4403	0.0000	0.001			
41:	4	3	1	3	2	1	10687.6480	-0.0002	0.001			
42:	4	3	2	3	2	2	10768.4335	-0.0002	0.001			
43:	4	4	0	3	3	0	11684.1763	0.0012	0.001			
44:	6	1	5	5	2	3	11355.5840	-0.0008	0.001			
45:	4	4	1	3	3	1	11686.2071	0.0005	0.001			
46:	7	2	6	6	3	4	11719.7341	0.0000	0.001			
47:	7	0	7	6	1	5	11774.1369	0.0043	0.003			
48:	5	1	4	4	0	4	11832.2547	0.0012	0.001			
49:	6	1	6	5	1	5	12035.6115	-0.0002	0.001			
50:	6	0	6	5	0	5	12071.4209	0.0000	0.001			
51:	6	2	5	5	2	4	12398.3401	0.0004	0.001			
52:	5	2	4	4	1	4	12398.4622	0.0016	0.001			
53:	6	3	4	5	3	3	12545.5810	-0.0003	0.001			
54:	6	4	3	5	4	2	12552.1668	-0.0001	0.001			
55:	6	1	5	5	1	4	12610.3065	-0.0002	0.001			
56:	6	3	3	5	3	2	12652.6773	-0.0007	0.001			
57:	5	3	2	4	2	2	12705.8911	0.0006	0.001			
58:	6	2	4	5	2	3	12806.1316	0.0002	0.001			
59:	5	3	3	4	2	3	12913.6964	-0.0003	0.001			
60:	7	2	5	6	3	3	13031.1548	-0.0010	0.001			
61:	7	1	6	6	2	4	13148.0979	0.0000	0.001			
62:	5	4	1	4	3	1	13763.8816	0.0003	0.001			
63:	7	0	7	6	0	6	14029.9673	-0.0002	0.001			
64:	6	2	4	5	1	4	14060.8534	0.0001	0.001			
65:	6	1	5	5	0	5	14327.2561	0.0002	0.001			
66:	7	2	6	6	2	5	14419.6314	-0.0003	0.001			
67:	7	1	6	6	1	5	14598.6441	-0.0003	0.001			
68:	7	3	5	6	3	4	14628.5591	0.0001	0.001			

69:	7	5	2	6	5	1	14640.0507	-0.0010	0.001
70:	7	5	3	6	5	2	14639.1251	0.0012	0.001
71:	7	4	4	6	4	3	14658.5093	-0.0003	0.001
72:	7	4	3	6	4	2	14681.4509	-0.0005	0.001
73:	6	3	3	5	2	3	14709.1291	0.0008	0.001
74:	5	5	0	4	4	0	14725.6818	0.0048	0.003
75:	5	5	1	4	4	1	14725.8648	-0.0021	0.001
76:	6	2	5	5	1	5	14743.1404	-0.0004	0.001
77:	8	1	7	7	2	5	14769.3994	0.0009	0.001
78:	7	3	4	6	3	3	14835.8560	0.0006	0.001
79:	7	2	5	6	2	4	14934.1534	0.0007	0.001
80:	6	3	4	5	2	4	15098.2367	-0.0006	0.001
81:	6	4	2	5	3	2	15825.4325	0.0001	0.001
82:	6	4	3	5	3	3	15875.7170	0.0000	0.001
83:	8	1	8	7	1	7	15982.9371	-0.0002	0.001
84:	8	0	8	7	0	7	15992.0798	-0.0003	0.001
85:	8	2	7	7	2	6	16425.6396	-0.0011	0.001
86:	7	2	5	6	1	5	16384.6987	-0.0005	0.001
87:	7	3	4	6	2	4	16738.8521	-0.0001	0.001
88:	6	5	1	5	4	1	16811.5954	0.0012	0.001
89:	6	5	2	5	4	2	16813.2493	0.0004	0.001
90:	6	6	0	5	5	0	17766.2567	0.0077	0.003
91:	6	6	1	5	5	1	17766.2642	-0.0007	0.001
92:	7	6	1	6	5	1	19853.2940	0.0063	0.003
93:	7	6	2	6	5	2	19853.4575	-0.0015	0.001
94:	8	4	4	7	3	4	19843.0701	-0.0005	0.001
95:	8	3	6	7	2	6	19607.1643	-0.0004	0.001
96:	8	2	7	7	1	7	19541.5522	0.0001	0.001
97:	8	1	7	7	0	7	19379.9650	-0.0001	0.001
98:	7	5	2	6	4	2	18892.2974	0.0010	0.001
99:	7	5	3	6	4	3	18900.2061	0.0004	0.001
100:	8	3	5	7	2	5	18836.1813	0.0001	0.001
101:	8	2	6	7	1	6	18809.1778	0.0002	0.001
102:	9	3	7	8	3	6	18751.7124	-0.0004	0.001
103:	7	4	4	6	3	4	17988.6447	-0.0006	0.001
104:	7	4	3	6	3	3	17854.2054	-0.0004	0.001
105:	7	2	6	6	1	6	17127.1608	0.0000	0.001
106:	8	3	5	7	3	4	17031.4833	0.0016	0.001
107:	5	1	5	4	0	4	10186.6568	-0.0007	0.001
108:	5	0	5	4	1	4	9982.3059	-0.0002	0.001
109:	6	0	6	5	1	5	12000.0675	-0.0001	0.001
110:	6	1	6	5	0	5	12106.9643	-0.0006	0.001
111:	7	0	7	6	1	6	13994.4233	-0.0001	0.001
112:	7	1	7	6	0	6	14046.7933	-0.0002	0.001
113:	4	0	4	3	1	3	7929.8120	0.0000	0.001
114:	4	1	4	3	0	3	8286.1265	0.0003	0.001

PARAMETERS IN FIT (values truncated):

10000	A	/MHz	1520.225823(64)	1
20000	B	/MHz	1097.367672(38)	2
30000	C	/MHz	983.704765(34)	3
200	DelJ	/kHz	0.04410(36)	4
1100	DelJK	/kHz	-0.0293(17)	5
2000	DelK	/kHz	0.0566(20)	6
40100	delJ	/kHz	0.00625(22)	7
41000	delK	/kHz	0.1363(26)	8

MICROWAVE AVG = 0.000236 MHz, IR AVG = 0.00000
MICROWAVE RMS = 0.001549 MHz, IR RMS = 0.00000
END OF ITERATION 1 OLD, NEW RMS ERROR= 0.95226 0.95226

distinct frequency lines in fit: 114
distinct parameters of fit: 8

	upper state		lower state		overall	
limits of quantum number 1:	1	9	0	8	0	9
limits of quantum number 2:	0	6	0	5	0	6
limits of quantum number 3:	0	8	0	7	0	8

frequency range: 2617 19853

Standard errors are obtained by muliplying the previous errors by: 0.987541

PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:
(values rounded)

10000	A	/MHz	1520.225823(63)	1
20000	B	/MHz	1097.367672(37)	2
30000	C	/MHz	983.704765(33)	3
200	DelJ	/kHz	0.04410(35)	4
1100	DelJK	/kHz	-0.0294(17)	5
2000	DelK	/kHz	0.0567(20)	6
40100	delJ	/kHz	0.00626(22)	7
41000	delK	/kHz	0.1364(26)	8

CORRELATION COEFFICIENTS, C.ij:

	A	B	C	-DelJ	-DelJK	-DelK	-delJ	-delK
A	1.0000							
B	-0.1076	1.0000						
C	0.2233	-0.0295	1.0000					
-DelJ	0.0389	-0.5931	-0.4649	1.0000				
-DelJK	-0.3986	0.1935	0.0113	-0.6314	1.0000			
-DelK	-0.2406	0.0355	-0.0450	0.3607	-0.6878	1.0000		
-delJ	0.1969	-0.6328	0.6490	0.0030	-0.0912	-0.0221	1.0000	
-delK	-0.0017	-0.0920	-0.0481	0.5778	-0.5520	0.3562	-0.1761	1.0000

Mean value of |C.ij|, i.ne.j = 0.2665
Mean value of C.ij, i.ne.j = -0.0774

No correlations with absolute value greater than 0.9950

Worst fitted lines (obs-calc/error):

30:	2.8	21:	-2.7	15:	-2.7	90:	2.6	
92:	2.1	12:	2.1	75:	-2.1	29:	2.0	
16:	1.8	17:	-1.7	106:	1.6	52:	1.6	
74:	1.6	93:	-1.5	47:	1.4	14:	1.4	
18:	1.3	48:	1.2	43:	1.2	36:	1.2	
27:	1.2	88:	1.2	70:	1.2	85:	-1.1	
60:	-1.0	24:	-1.0	69:	-1.0	98:	1.0	
2:	-0.9	3:	-0.9	77:	0.9	19:	0.9	
20:	-0.8	44:	-0.8	35:	0.8	73:	0.8	
28:	-0.7	107:	-0.7	25:	0.7	91:	-0.7	
79:	0.7	56:	-0.7	103:	-0.6	80:	-0.6	
78:	0.6	57:	0.6	110:	-0.6	86:	-0.5	
13:	-0.5	72:	-0.5					

30:	6	2	5	5	3	3	9845.6865	0.0028	0.001
21:	2	1	1	1	0	1	4812.3238	-0.0027	0.001
15:	4	0	4	3	1	2	7250.0758	-0.0027	0.001
90:	6	6	0	5	5	0	17766.2567	0.0077	0.003
92:	7	6	1	6	5	1	19853.2940	0.0063	0.003
12:	3	2	1	2	1	1	7607.9645	0.0021	0.001
75:	5	5	1	4	4	1	14725.8648	-0.0021	0.001
29:	6	1	6	5	2	4	9690.8126	0.0020	0.001
16:	3	2	1	2	2	0	6319.4021	0.0055	0.003
17:	3	2	2	2	2	1	6243.2115	-0.0017	0.001

EXO-Fenchol- 1XF

							obs	o-c	error	blends o-c	blends wt	Notes
/ instead of : below denotes (o-c)>3*err												
1:	4	1	4	3	1	3	7622.9414	-0.0005	0.002			
2:	3	0	3	2	0	2	5877.3380	-0.0007	0.002			
3:	3	1	3	2	1	2	5786.6440	-0.0030	0.002			
4:	6	1	6	5	1	5	11244.1739	0.0002	0.002			
5:	6	0	6	5	0	5	11246.3191	0.0004	0.002			
6:	5	1	5	4	1	4	9437.5136	0.0002	0.002			
7:	7	0	7	6	0	6	13049.0555	0.0000	0.002			
8:	7	1	7	6	1	6	13048.5699	0.0000	0.002			
9:	8	1	8	7	1	7	14852.4290	0.0000	0.002			
10:	8	0	8	7	0	7	14852.5333	-0.0004	0.002			
11:	4	2	3	3	2	2	8298.9616	0.0000	0.002			
12:	3	1	2	2	1	1	6639.0847	-0.0007	0.002			
13:	3	2	1	2	1	1	7765.2169	-0.0023	0.002			
14:	4	1	3	3	1	2	8589.9285	0.0007	0.002			
15:	4	2	2	3	2	1	9045.9391	-0.0001	0.002			
16:	5	0	5	4	0	4	9446.3212	-0.0003	0.002			
17:	5	2	4	4	2	3	10211.3613	0.0051	0.002			
18:	5	1	4	4	1	3	10378.0248	-0.0004	0.002			
19:	5	3	3	4	3	2	10704.1587	-0.0006	0.002			
20:	5	3	2	4	3	1	11259.9634	0.0008	0.002			
21:	6	1	5	5	1	4	12131.4611	-0.0003	0.002			
22:	6	2	5	5	2	4	12065.8572	0.0001	0.002			
23:	6	3	4	5	3	3	12720.0527	-0.0002	0.002			
24:	5	3	2	4	2	2	12815.8282	-0.0009	0.002			
25:	7	2	5	6	2	4	14887.3634	-0.0003	0.002			
26:	7	2	6	6	2	5	13888.1055	0.0003	0.002			
27:	6	3	3	5	3	2	13603.0250	-0.0012	0.002			
28:	4	3	2	3	2	2	10896.7443	-0.0011	0.002			
29:	4	3	1	3	2	1	10601.8091	0.0032	0.002			
30:	4	2	2	3	1	2	10172.0732	0.0001	0.002			
31:	4	4	0	3	3	0	11523.0149	0.0002	0.002			
32:	4	4	1	3	3	1	11557.2938	0.0002	0.002			
33:	4	4	0	3	3	1	11570.2920	-0.0003	0.002			
34:	4	4	1	3	3	0	11510.0155	-0.0004	0.002			
35:	5	0	5	4	1	4	9434.7510	0.0001	0.002			
36:	6	1	6	5	0	5	11246.9358	-0.0003	0.002			
37:	6	0	6	5	1	5	11243.5562	0.0000	0.002			
38:	5	2	3	4	2	2	11192.2311	-0.0002	0.002			
39:	5	2	3	4	1	3	12774.3777	0.0010	0.002			
40:	4	1	4	3	0	3	7666.4578	0.0001	0.002			
41:	4	0	4	3	1	3	7611.3714	0.0001	0.002			
42:	4	0	4	3	0	3	7654.8869	0.0000	0.002			

PARAMETERS IN FIT (values truncated):

10000	A	/MHz	1494.88444(46)	1
20000	B	/MHz	1201.81174(20)	2
30000	C	/MHz	901.90593(11)	3
200	DELTA J	/kHz	0.0285(18)	4
2000	DELTA K	/kHz	0.034(21)	5
40100	delta J	/kHz	0.0062(10)	6

MICROWAVE AVG = -0.000041 MHz, IR AVG = 0.00000
MICROWAVE RMS = 0.001217 MHz, IR RMS = 0.00000
END OF ITERATION 1 OLD, NEW RMS ERROR= 0.60873 0.60873

distinct frequency lines in fit: 42
distinct parameters of fit: 6

	upper state		lower state		overall	
limits of quantum number 1:	3	8	2	7	2	8
limits of quantum number 2:	0	4	0	3	0	4
limits of quantum number 3:	0	8	0	7	0	8

frequency range: 5786 14887

Standard errors are obtained by muliplying the previous errors by: 0.657504

PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:
(values rounded)

10000	A	/MHz	1494.88444(30)	1
20000	B	/MHz	1201.81175(13)	2
30000	C	/MHz	901.905933(74)	3
200	DELTA J	/kHz	0.0285(12)	4
2000	DELTA K	/kHz	0.035(14)	5
40100	delta J	/kHz	0.00626(71)	6

Worst fitted constants, with greater than 20% uncertainty: %

2000	DELTA K	/kHz	0.035(14)	5	40.2

CORRELATION COEFFICIENTS, C.ij:

	A	B	C	-DELTA J	-DELTA K	-delta J
A	1.0000					
B	-0.2161	1.0000				
C	-0.1222	-0.0111	1.0000			
-DELTA J	0.1979	-0.8245	-0.4052	1.0000		
-DELTA K	-0.9546	0.2938	0.1528	-0.3224	1.0000	
-delta J	0.1644	-0.8688	0.1985	0.7817	-0.2681	1.0000

Mean value of |C.ij|, i.ne.j = 0.3855
Mean value of C.ij, i.ne.j = -0.1469

No correlations with absolute value greater than 0.9950

Worst fitted lines (obs-calc/error):

17:	2.6	29:	1.6	3:	-1.5	13:	-1.1				
27:	-0.6	28:	-0.6	39:	0.5	24:	-0.4				
20:	0.4	14:	0.3	12:	-0.3	2:	-0.3				
19:	-0.3	1:	-0.2	18:	-0.2	5:	0.2				
10:	-0.2	34:	-0.2	26:	0.1	33:	-0.1				
25:	-0.1	21:	-0.1	16:	-0.1	36:	-0.1				
32:	0.1	31:	0.1	4:	0.1	38:	-0.1				
23:	-0.1	6:	0.1	22:	0.1	41:	0.1				
40:	0.1	15:	-0.1	35:	0.1	30:	0.1				
42:	0.0	37:	0.0	11:	0.0	9:	0.0				
8:	0.0	7:	0.0								

17:	5	2	4	4	2	3	10211.3613	0.0051	0.002
29:	4	3	1	3	2	1	10601.8091	0.0032	0.002
3:	3	1	3	2	1	2	5786.6440	-0.0030	0.002
13:	3	2	1	2	1	1	7765.2169	-0.0023	0.002
27:	6	3	3	5	3	2	13603.0250	-0.0012	0.002
28:	4	3	2	3	2	2	10896.7443	-0.0011	0.002
39:	5	2	3	4	1	3	12774.3777	0.0010	0.002
24:	5	3	2	4	2	2	12815.8282	-0.0009	0.002
20:	5	3	2	4	3	1	11259.9634	0.0008	0.002
14:	4	1	3	3	1	2	8589.9285	0.0007	0.002

ENDO-Fenchol-OD

									obs	o-c	error	blends o-c	blends wt	Notes
/ instead of : below denotes (o-c)>3*err														
1/	3	1	3	4	2	1	2	3	5997.3565	0.0000	0.002	-0.0062	0.33	
2:	3	1	3	2	2	1	2	1	5997.3565	-0.0078	0.002	-0.0062	0.33	
3:	3	1	3	3	2	1	2	2	5997.3565	-0.0106	0.002	-0.0062	0.33	
4:	3	0	3	4	2	0	2	3	6103.6638	0.0013	0.002			
5:	3	0	3	2	2	0	2	1	6103.6646	0.0014	0.002			
6:	3	2	2	2	2	2	1	1	6196.5435	0.0000	0.002			
7:	3	2	2	4	2	2	1	3	6196.5598	0.0050	0.002			
8:	3	2	2	3	2	2	1	2	6196.5710	-0.0039	0.002			
9:	3	1	2	4	2	1	1	3	6364.2786	-0.0007	0.002			
10:	3	1	2	3	2	1	1	2	6364.2873	-0.0004	0.002			
11:	4	1	4	5	3	1	3	4	7974.0148	-0.0002	0.002			
12:	4	1	4	3	3	1	3	2	7974.0231	0.0038	0.002	0.0019	0.50	
13:	4	1	4	4	3	1	3	3	7974.0231	0.0000	0.002	0.0019	0.50	
14:	4	0	4	5	3	0	3	4	8058.3043	0.0016	0.002	0.0015	0.50	
15:	4	0	4	3	3	0	3	2	8058.3043	0.0012	0.002	0.0015	0.50	
16:	4	2	3	3	3	2	2	2	8242.6644	-0.0020	0.002			
17:	4	2	3	3	3	2	2	3	8242.6690	0.0025	0.002			
18:	4	2	3	5	3	2	2	4	8242.6749	0.0055	0.002			
19:	4	2	2	3	3	2	1	2	8446.1051	0.0027	0.002			
20:	4	2	2	4	3	2	1	3	8446.1052	0.0051	0.002			
21:	4	2	2	5	3	2	1	4	8446.1096	0.0056	0.002			
22:	4	1	3	3	3	1	2	2	8448.9884	0.0038	0.002			
23:	4	1	3	5	3	1	2	4	8448.9885	-0.0010	0.002			
24:	4	1	3	4	3	1	2	3	8448.9970	-0.0020	0.002			
25:	5	1	5	6	4	1	4	5	9938.5140	0.0001	0.002			
26:	5	1	5	4	4	1	4	3	9938.5141	-0.0024	0.002			
27:	5	1	5	5	4	1	4	4	9938.5200	-0.0006	0.002			
28:	3	3	0	2	2	2	0	1	8468.7095	0.0022	0.002			
29:	3	3	0	3	2	2	0	2	8468.7133	-0.0020	0.002			
30:	3	3	0	4	2	2	0	3	8468.7153	0.0011	0.002			
31:	3	3	1	3	2	2	1	2	8490.2463	0.0053	0.002	0.0011	0.50	
32:	3	3	1	2	2	2	1	1	8490.2463	-0.0030	0.002	0.0011	0.50	
33:	3	3	1	4	2	2	1	3	8490.2475	-0.0027	0.002			
34:	4	2	2	4	3	1	2	3	9578.6459	-0.0016	0.002			
35:	4	2	2	3	3	1	2	2	9578.6520	0.0024	0.002	0.0016	0.50	
36:	4	2	2	5	3	1	2	4	9578.6520	0.0008	0.002	0.0016	0.50	
37:	5	2	3	4	4	2	2	3	10606.5577	-0.0056	0.002	-0.0051	0.50	
38:	5	2	3	5	4	2	2	4	10606.5577	-0.0044	0.002	-0.0051	0.50	
39:	5	2	3	6	4	2	2	5	10606.5637	-0.0008	0.002			
40:	4	3	2	4	3	2	2	3	10597.0788	-0.0036	0.002			
41:	4	3	2	5	3	2	2	4	10597.0989	0.0011	0.002			
42:	4	3	2	3	3	2	2	2	10597.1012	-0.0004	0.002			
43:	4	3	1	3	3	2	1	2	10501.1348	-0.0012	0.002			
44:	4	3	1	5	3	2	1	4	10501.1410	0.0004	0.002			
45:	4	3	1	4	3	2	1	3	10501.1470	-0.0010	0.002			
46:	5	2	4	4	4	2	3	3	10272.8852	-0.0009	0.002	-0.0015	0.50	
47:	5	2	4	6	4	2	3	5	10272.8852	-0.0021	0.002	-0.0015	0.50	
48:	5	2	4	5	4	2	3	4	10272.8949	-0.0015	0.002			
49:	5	1	4	4	4	1	3	3	10494.5173	0.0008	0.002	-0.0009	0.50	
50:	5	1	4	6	4	1	3	5	10494.5173	-0.0026	0.002	-0.0009	0.50	
51:	5	1	4	5	4	1	3	4	10494.5286	-0.0037	0.002			
52:	5	2	3	5	4	1	3	4	11736.2090	-0.0017	0.002			
53:	5	2	3	6	4	1	3	5	11736.2264	0.0002	0.002			
54:	5	2	3	4	4	1	3	3	11736.2281	-0.0002	0.002			
55:	4	4	1	4	3	3	1	3	11458.6633	0.0010	0.002			
56:	4	4	1	3	3	3	1	2	11458.6655	0.0016	0.002	0.0007	0.50	
57:	4	4	1	5	3	3	1	4	11458.6655	-0.0002	0.002	0.0007	0.50	
58:	4	4	0	4	3	3	0	3	11455.8312	-0.0006	0.002	-0.0007	0.50	
59:	4	4	0	3	3	3	0	2	11455.8312	-0.0007	0.002	-0.0007	0.50	
60:	4	4	0	5	3	3	0	4	11455.8359	0.0017	0.002			
61:	6	1	6	7	5	1	5	6	11893.6193	-0.0035	0.002			
62:	6	1	6	5	5	1	5	4	11893.6241	-0.0006	0.002			
63:	6	1	6	6	5	1	5	5	11893.6302	0.0015	0.002			
64:	6	0	6	7	5	0	5	6	11921.7173	0.0017	0.002			
65:	6	0	6	5	5	0	5	4	11921.7205	0.0037	0.002			
66:	6	0	6	6	5	0	5	5	11921.7226	-0.0015	0.002			
67:	6	2	4	5	5	2	3	4	12744.8247	-0.0029	0.002			
68:	6	2	4	7	5	2	3	6	12744.8317	0.0026	0.002			

69/	6	2	4	6	5	2	3	5	12744.8378	0.0073	0.002			
70:	5	3	3	5	4	2	3	4	12739.0901	-0.0001	0.002			
71:	5	3	3	6	4	2	3	5	12739.1128	0.0032	0.002			
72:	5	3	3	4	4	2	3	3	12739.1146	0.0005	0.002			
73:	6	3	3	6	5	3	2	5	12603.6458	-0.0033	0.002			
74:	6	3	3	5	5	3	2	4	12603.6526	-0.0016	0.002			
75:	6	3	3	7	5	3	2	6	12603.6553	0.0012	0.002			
76:	6	3	4	5	5	3	3	4	12459.6912	-0.0010	0.002	-0.0016	0.50	
77:	6	3	4	7	5	3	3	6	12459.6912	-0.0022	0.002	-0.0016	0.50	
78:	6	3	4	6	5	3	3	5	12459.6959	-0.0028	0.002			
79:	6	1	5	5	5	1	4	4	12489.5054	-0.0023	0.002	-0.0037	0.50	
80:	6	1	5	7	5	1	4	6	12489.5054	-0.0050	0.002	-0.0037	0.50	
81:	6	1	5	6	5	1	4	5	12489.5287	0.0032	0.002			
82:	5	4	1	5	4	3	1	4	13518.8648	-0.0026	0.002			
83:	5	4	1	4	4	3	1	3	13518.8731	0.0053	0.002	0.0049	0.50	
84:	5	4	1	6	4	3	1	5	13518.8731	0.0045	0.002	0.0049	0.50	
85:	7	1	7	8	6	1	6	7	13842.5514	-0.009	UNFITTD	13842.5604		
86:	7	1	7	6	6	1	6	5	13842.5618	0.0000	0.002	-0.0018	0.50	
87:	7	1	7	7	6	1	6	6	13842.5618	-0.0034	0.002	-0.0018	0.50	
88:	6	2	4	6	5	1	4	5	13986.5043	-0.0045	0.002			
89:	6	2	4	7	5	1	4	6	13986.5370	0.0017	0.002	-0.0004	0.50	
90:	6	2	4	5	5	1	4	4	13986.5370	-0.0024	0.002	-0.0004	0.50	
91:	7	0	7	8	6	0	6	7	13856.0809	0.0011	0.002	0.0005	0.50	
92:	7	0	7	6	6	0	6	5	13856.0809	-0.0001	0.002	0.0005	0.50	
93:	7	0	7	7	6	0	6	6	13856.0855	-0.0004	0.002			
94:	6	1	5	7	5	0	5	6	14309.7297	-0.0018	0.002			
95:	5	5	0	5	4	4	0	4	14434.5990	0.0026	0.002	0.0017	0.33	
96:	5	5	0	4	4	4	0	3	14434.5990	0.0019	0.002	0.0017	0.33	
97:	5	5	0	6	4	4	0	5	14434.5990	0.0006	0.002	0.0017	0.33	
98:	5	5	1	5	4	4	1	4	14434.8987	-0.0008	0.002	-0.0019	0.33	
99:	5	5	1	4	4	4	1	3	14434.8987	-0.0016	0.002	-0.0019	0.33	
100:	5	5	1	6	4	4	1	5	14434.8987	-0.0030	0.002	-0.0019	0.33	
101:	7	1	6	6	6	1	5	5	14437.4063	0.0014	0.002			
102:	7	1	6	8	6	1	5	7	14437.4070	0.0002	0.002			
103:	7	1	6	7	6	1	5	6	14437.4182	-0.0038	0.002			
105:	7	3	5	6	6	3	4	5	14522.3402	0.0022	0.002	0.0018	0.50	
106:	7	3	5	8	6	3	4	7	14522.3402	0.0014	0.002	0.0018	0.50	
107:	7	3	4	7	6	3	3	6	14789.3080	0.0037	0.002	-0.0004	0.33	
108:	7	3	4	8	6	3	3	7	14789.3080	-0.0023	0.002	-0.0004	0.33	
109:	7	3	4	6	6	3	3	5	14789.3080	-0.0026	0.002	-0.0004	0.33	
110:	7	2	5	6	6	2	4	5	14844.7803	0.0050	0.002	0.0043	0.50	
111:	7	2	5	8	6	2	4	7	14844.7803	0.0035	0.002	0.0043	0.50	
112:	6	3	4	6	5	2	4	5	14925.8915	-0.0011	0.002			
113:	6	3	4	7	5	2	4	6	14925.9209	0.0052	0.002	0.0030	0.50	
114:	6	3	4	5	5	2	4	4	14925.9209	0.0006	0.002	0.0030	0.50	
115:	6	4	2	7	5	3	2	6	15558.4674	-0.0006	0.002	-0.0023	0.50	
116:	6	4	2	6	5	3	2	5	15558.4674	-0.0039	0.002	-0.0023	0.50	
117:	6	4	3	7	5	3	3	6	15626.4270	-0.0020	0.002			
118:	6	4	3	5	5	3	3	4	15626.4327	0.0028	0.002			
119:	8	1	8	9	7	1	7	8	15787.9535	0.0024	0.002	0.0008	0.33	
120:	8	1	8	7	7	1	7	6	15787.9535	0.0012	0.002	0.0008	0.33	
121:	8	1	8	8	7	1	7	7	15787.9535	-0.0015	0.002	0.0008	0.33	
122:	8	0	8	9	7	0	7	8	15794.0550	0.0018	0.002	0.0000	0.33	
123:	8	0	8	7	7	0	7	6	15794.0550	0.0007	0.002	0.0000	0.33	
124:	8	0	8	8	7	0	7	7	15794.0550	-0.0026	0.002	0.0000	0.33	
125:	9	1	9	10	8	1	8	9	17731.5062	-0.0053	0.002			
126:	9	1	9	8	8	1	8	7	17731.5100	-0.0025	0.002			
127:	9	1	9	9	8	1	8	8	17731.5208	0.0059	0.002			
128:	9	0	9	10	8	0	8	9	17734.1494	0.0000	0.002	-0.0005	0.50	
129:	9	0	9	8	8	0	8	7	17734.1494	-0.0009	0.002	-0.0005	0.50	
130:	10	1	10	11	9	1	9	10	19674.2073	0.0022	0.002	0.0010	0.33	
131:	10	1	10	9	9	1	9	8	19674.2073	0.0014	0.002	0.0010	0.33	
132:	10	1	10	10	9	1	9	9	19674.2073	-0.0005	0.002	0.0010	0.33	
133:	10	0	10	11	9	0	9	10	19675.3125	0.0020	0.002	0.0008	0.33	
134:	10	0	10	9	9	0	9	8	19675.3125	0.0011	0.002	0.0008	0.33	
135:	10	0	10	10	9	0	9	9	19675.3125	-0.0008	0.002	0.0008	0.33	
136:	6	3	3	6	5	2	3	5	14497.5835	-0.0025	0.002	0.0021	0.50	
137:	6	3	3	7	5	2	3	6	14497.5835	0.0067	0.002	0.0021	0.50	
138:	5	4	2	5	4	3	2	4	13537.5307	-0.0025	0.002			
139:	5	4	2	6	4	3	2	5	13537.5348	-0.0037	0.002			
140:	5	4	2	4	4	3	2	3	13537.5403	0.0014	0.002			
141:	7	2	6	6	6	2	5	5	14278.4438	0.0015	0.002	0.0013	0.50	
142:	7	2	6	8	6	2	5	7	14278.4438	0.0011	0.002	0.0013	0.50	
143:	5	3	3	5	4	2	3	4	12739.0901	-0.0001	0.002			
144:	5	3	3	6	4	2	3	5	12739.1128	0.0032	0.002			

```
 145:  5  3  3  4    4  2  3  3             12739.1146   0.0005  0.002
-------------------------------------------------------------------------------------------=========
    1 Lines rejected from fit

PARAMETERS IN FIT (values truncated):

       10000            A  /MHz         1488.66758(24)                          1
       20000            B  /MHz         1094.44231(19)                          2
       30000            C  /MHz          971.07905(12)                          3
         200         DelJ  /kHz            0.0486(18)                          4
        1100        DelJK  /kHz           -0.014(11)                           5
        2000         DelK  /kHz            0.035(12)                           6
       40100         delJ  /kHz            0.00698(93)                         7
       41000         delK  /kHz            0.160(17)                           8
   110010000   3/2*Chi_aa  /MHz            0.0941(80)                          9
   110040000   1/4*(Chi_b  /MHz            0.0719(38)                         10

 MICROWAVE AVG =        0.000020 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.002636 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        1.31796         1.31796

  distinct frequency lines in fit:   105
       distinct parameters of fit:    10
          lines rejected from fit:     1

                                    upper state  lower state         overall
      limits of quantum number  1:      3   10       2    9           2   10
      limits of quantum number  2:      0    5       0    4           0    5
      limits of quantum number  3:      0   10       0    9           0   10
      limits of quantum number  4:      2   11       1   10           1   11

                  frequency range:        5997        19675

 FRAC<0 was used so that the errors above are  1.0000 times the standard error

 PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:
(values rounded)

       10000            A  /MHz         1488.66758(24)                          1
       20000            B  /MHz         1094.44232(19)                          2
       30000            C  /MHz          971.07906(12)                          3
         200         DelJ  /kHz            0.0486(18)                          4
        1100        DelJK  /kHz           -0.015(11)                           5
        2000         DelK  /kHz            0.035(12)                           6
       40100         delJ  /kHz            0.00698(93)                         7
       41000         delK  /kHz            0.161(17)                           8
   110010000   3/2*Chi_aa  /MHz            0.0941(80)                          9
   110040000   1/4*(Chi_b  /MHz            0.0719(38)                         10

-------------------------------------------------------------------------------------------
 Worst fitted constants, with greater than 20% uncertainty:                              %

        1100        DelJK  /kHz           -0.015(11)                           5      74.7
        2000         DelK  /kHz            0.035(12)                           6      34.7
-------------------------------------------------------------------------------------------

 CORRELATION COEFFICIENTS, C.ij:

           A        B        C        -DelJ    -DelJK   -DelK    -delJ    -delK

A           1.0000
B          -0.1479   1.0000
C           0.0352  -0.3941   1.0000
-DelJ       0.2083  -0.8709   0.3037   1.0000
-DelJK     -0.4537   0.4190  -0.4257  -0.6957   1.0000
-DelK      -0.2019  -0.1489   0.3262   0.4069  -0.7132   1.0000
-delJ       0.2129  -0.9090   0.4791   0.9064  -0.6083   0.3289   1.0000
-delK       0.0054  -0.5243   0.6842   0.6505  -0.6046   0.4505   0.5301   1.0000
3/2*Chi_aa  0.0055   0.0343   0.0018  -0.0314   0.0124  -0.0072  -0.0247  -0.0172
1/4*(Chi_b  0.0143  -0.1656   0.1953   0.1424  -0.1128   0.0658   0.1519   0.2001

           3/2*Chi_ 1/4*(Chi

3/2*Chi_aa  1.0000
1/4*(Chi_b -0.0081   1.0000
```

Mean value of |C.ij|, i.ne.j = 0.3075
Mean value of C.ij, i.ne.j = -0.0065

No correlations with absolute value greater than 0.9950

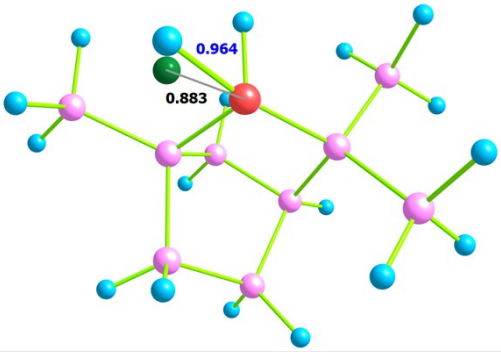
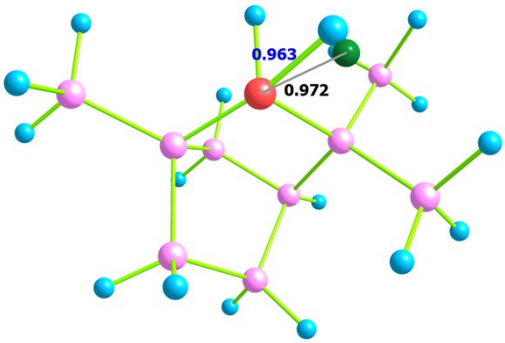
Worst fitted lines (obs-calc/error):

69:	3.6	1:	-3.1	127:	2.9	21:	2.8
18:	2.8	125:	-2.6	20:	2.6	37:	-2.5
7:	2.5	83:	2.5	88:	-2.2	110:	2.1
8:	-1.9	22:	1.9	103:	-1.9	79:	-1.9
139:	-1.9	51:	-1.9	65:	1.9	40:	-1.8
61:	-1.8	73:	-1.6	81:	1.6	144:	1.6
71:	1.6	113:	1.5	67:	-1.4	78:	-1.4
118:	1.4	33:	-1.4	19:	1.4	68:	1.3
82:	-1.3	126:	-1.2	17:	1.2	138:	-1.2
26:	-1.2	115:	-1.1	28:	1.1	136:	1.0
117:	-1.0	29:	-1.0	24:	-1.0	16:	-1.0
12:	1.0	98:	-0.9	105:	0.9	94:	-0.9
86:	-0.9	95:	0.9				

69/	6	2	4	6	5	2	3	5	12744.8378	0.0073	0.002	
1/	3	1	3	4	2	1	2	3	5997.3565	0.0000	0.002	-0.0062 0.33
127:	9	0	9	10	8	0	8	9	17734.1494	0.0000	0.002	-0.0005 0.50
21:	4	2	2	5	3	2	1	4	8446.1096	0.0056	0.002	
18:	4	2	3	5	3	2	2	4	8242.6749	0.0055	0.002	
125:	9	1	9	8	8	1	8	7	17731.5100	-0.0025	0.002	
20:	4	2	2	4	3	2	1	3	8446.1052	0.0051	0.002	
37:	5	2	3	4	4	2	2	3	10606.5577	-0.0056	0.002	-0.0051 0.50
7:	3	2	2	4	2	2	1	3	6196.5598	0.0050	0.002	
83:	5	4	1	4	4	3	1	3	13518.8731	0.0053	0.002	0.0049 0.50

SPFIT output reformatted with PIFORM

Rs structure: Position of the D atom (in green) compared to the calculated molecular structure.

1EF	2EF
	

Calculated values of the diagonal elements for the spin-spin tensors associated with the three methylene group of endo-fenchol (C(5)H2, C(6)H2, C(7)H2)

These values reproduce the signals presented in Figure 4.

C(5)H2: 3/2Daa = -5.46 kHz ; 3/2Dbb = -12.3 kHz; 3/2Dcc = 17.8 kHz
C(6)H2: 3/2Daa = -4.1 kHz ; 3/2Dbb = -1.94 kHz; 3/2Dcc = 6.05 kHz
C(7)H2: 3/2Daa = 6.19 kHz; 3/2Dbb = -11.58 kHz ; 3/2Dcc = 5.35 kHz

Table 1. The calculated values of molecular parameters presented in the Table 2 of the paper

Endo-fenchol	1EF[a]	1EF[b]	2EF[a]	2EF[b]
A/MHz	1524.3	1533.0	1527.2	1535.1
B/MHz	1108.3	1115.6	1102.3	1110.4
C/MHz	984.9	991.8	989.6	995.7
Δ_J/kHz	0.03715	-	0.03970	-
Δ_{JK}/kHz	-0.0369	-	-0.0497	-
Δ_K/kHz	0.0588	-	0.0713	-
δ_J/kHz	0.00500	-	0.00531	-
δ_K/kHz	0.0779	-	0.1045	-
$\lvert\mu_a\rvert$/D	1.2	1.1	1.1	1.0
$\lvert\mu_b\rvert$/D	0.02	0.03	0.04	0.06
$\lvert\mu_c\rvert$/D	1.1	1.1	1.0	0.94
Exo-fenchol	1XF[a]	1XF[b]	2XF[a]	2XF[b]
A/MHz	1500.3	1519.3	1502.0	1510.6
B/MHz	1209.2	1091.7	1211.1	1218.9
C/MHz	906.9	977.9	907.5	913.2
Δ_J/kHz	0.0483	-	0.0477	-
Δ_{JK}/kHz	-0.0561	-	-0.0572	-
Δ_K/kHz	0.0232	-	0.0252	-
δ_J/kHz	0.0036	-	0.0036	-
δ_K/kHz	0.023	-	0.024	-
$\lvert\mu_a\rvert$/D	1.2	1.0	1.3	1.1
$\lvert\mu_b\rvert$/D	0.7	0.6	0.8	0.6
$\lvert\mu_c\rvert$/D	0.8	0.7	0.6	0.5

[a] MP2/6-311++G(d,p) basis set ; [b] MP2/aug-cc-pVTZ basis set.