Supporting information:

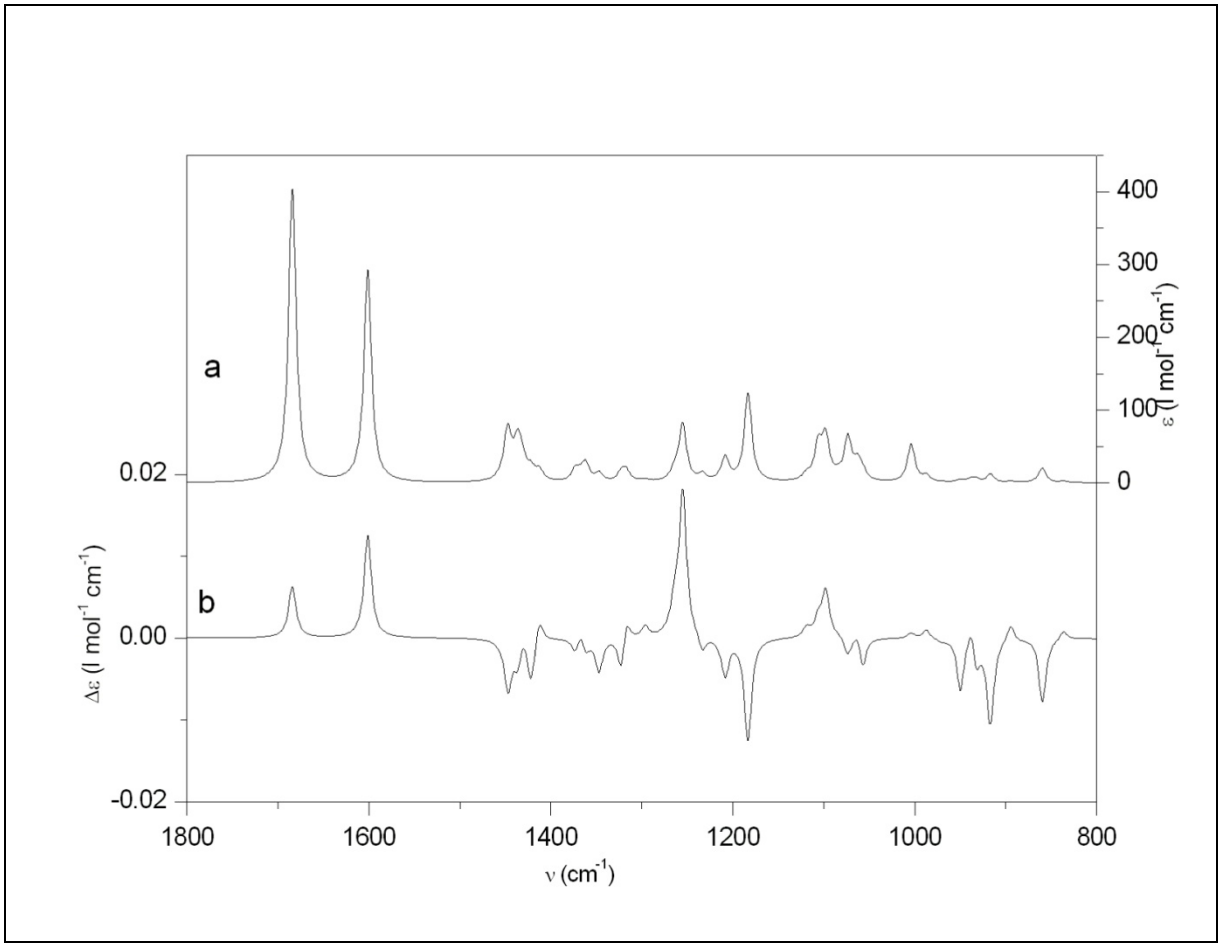

Figure S1: The calculated IR (a) and VCD (b) spectra of R – pulegone, using a cc – pVTZ basis set. In order to scale the frequencies, a scaling factor of 0.965 was used.

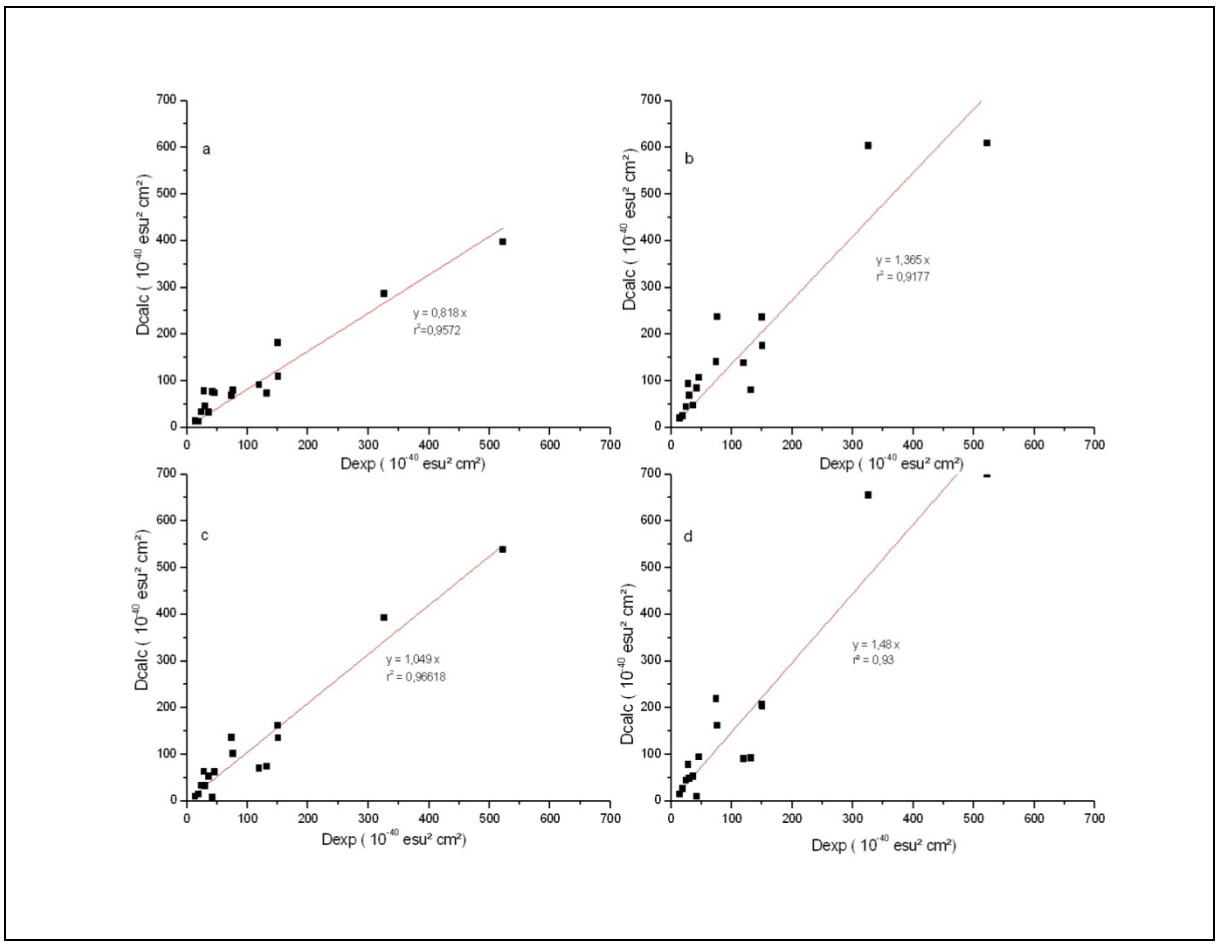

Figure S2: Comparison of the experimental Dipole strengths and the calculated ones: (a) calculations of pulegone in vacuum, (b) PCM calculations of pulegone, (c) calculations of the 1:1 pulegone.$CDCl_3$ associations and (d) PCM calculations of the complexes.

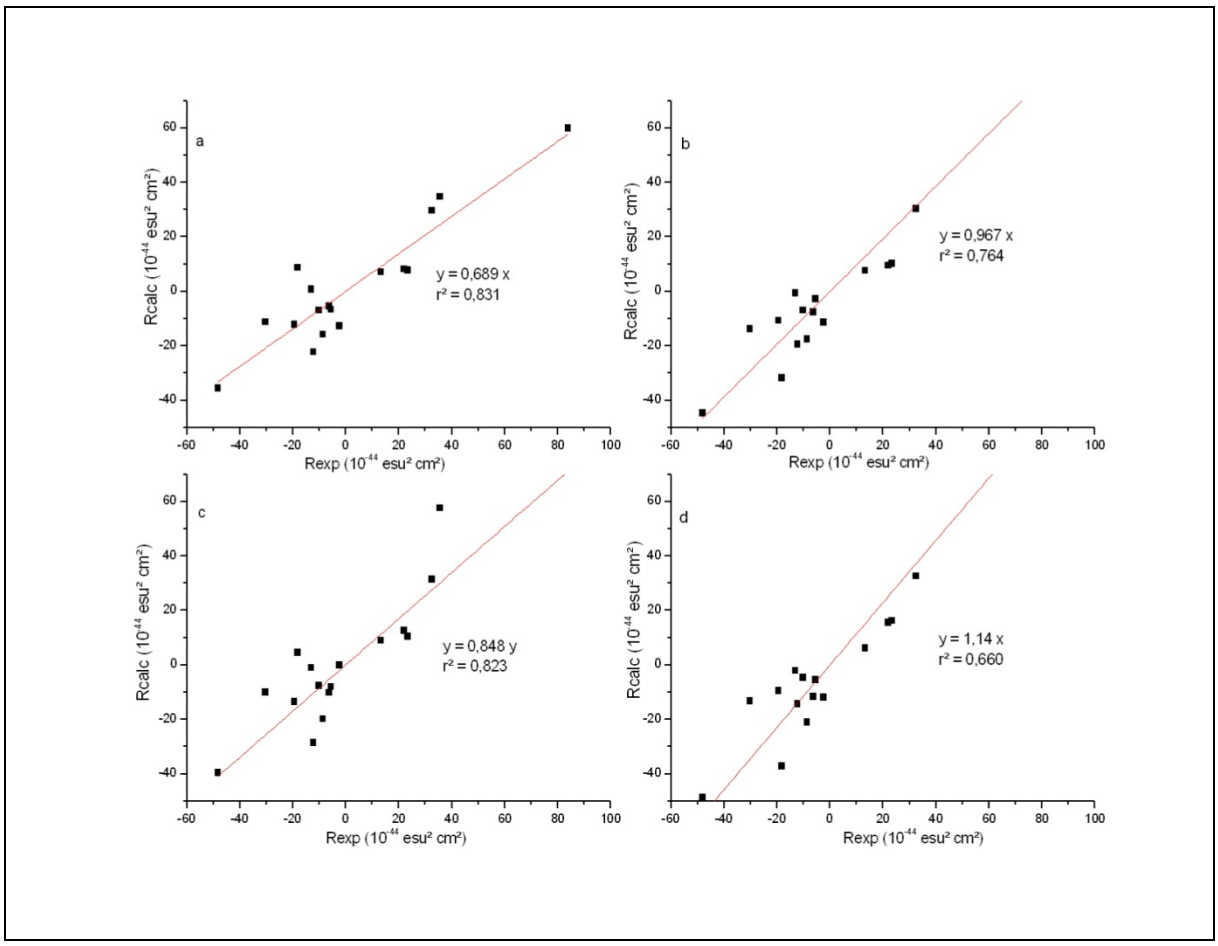

Figure S3: Comparison of the experimental Rotational strengths and the calculated ones: (a) calculations of R - pulegone in vacuum, (b) PCM calculations of R - pulegone, (c) calculations of the 1:1 R - pulegone.$CDCl_3$ associations and (d) PCM calculations of the complexes.

Table S1: A quantitative comparison of the experimental and theoretical Rotational and Dipole strengths of each normal mode from 1000 cm^{-1} till 1800 cm^{-1}. D values in 10^{-40} esu^2 cm^2, R values in 10^{-44} esu^2 cm^2 and frequencies in cm^{-1}. The calculations in vacuum and PCM calculations in $CHCl_3$ were compared to the experiment. The notation *a* refers to the equatorial conformer, *b* to the axial conformer.

	Experimental			B3LYP/6-311+G**			PCM		
Fund	Freq	D	R	Freq	D	R	Freq	D	R
29a	1013	14.13	23.33	988	10.70	4.00	985	16.35	8.82
30b				988	2.82	1.35	988	3.59	1.18
30a	1030	45.86		1005	73.86	2.40	1004	107.09	0.15
31b	1063	29.94	-8.64	1053	0.43	0.86	1051	1.26	1.10
31a				1056	17.22	-16.64	1054	20.05	-18.67
32b	1079		22.04	1060	6.21	1.16	1057	7.85	1.06
32a				1062	21.19	7.73	1060	38.75	9.24
33b				1065	0.64	-0.76	1063	0.40	-0.80
33a	1096	28.42	-5.55	1073	70.59	-7.84	1072	84.18	-4.04

34b				1086	7.76	1.21	1083	9.25	1.36
34a	1128	74.39	32.59	1100	69.03	18.65	1098	140.71	16.75
35b	1140	42.49		1102	3.21	-1.78	1100	4.67	-1.69
35a				1107	63.82	8.69	1105	67.81	11.62
36a				1118	7.92	4.04	1116	10.36	3.52
36b				1122	1.39	0.05	1120	1.69	0.15
37b	1212	149.89	-48.19	1183	6.94	0.34	1180	7.83	-0.66
37a				1184	137.56	-35.73	1185	189.88	-44.38
38b				1194	0.22	-0.22	1193	0.87	0.35
38a	1229		-19.44	1209	36.05	-11.62	1206	36.90	-10.12
39b				1217	0.77	-0.58	1213	1.56	-0.59
39a	1273	19.36	-10.13	1234	13.11	-6.90	1230	25.29	-6.95
40a	1288	150.82	83.88	1256	84.09	51.07	1255	139.43	58.57
40b				1257	7.52	-1.94	1257	9.63	-2.32
41a				1265	17.32	10.34	1264	26.43	15.47
41b				1274	0.12	0.38	1270	0.31	0.50
42a	1336	24.74	-13.02	1295	2.38	3.82	1292	3.75	3.51
42b				1303	0.87	0.04	1300	0.87	0.05
43a				1317	14.11	9.39	1314	18.35	8.28
43b				1323	0.95	0.78	1321	1.34	0.83
44a				1323	14.67	-13.61	1319	19.88	-13.48
44b				1334	0.15	0.29	1332	0.16	0.33
45b	1373	132.11	-30.25	1340	0.10	-0.58	1338	0.07	-0.45
45a				1348	13.89	-10.64	1345	15.76	-13.35
46b	1385		-6.21	1362	1.87	0.27	1359	1.91	0.23
46a				1362	24.90	-7.00	1359	30.64	-6.27
47a				1366	12.08	5.69	1363	9.04	5.82
47b				1370	1.46	-0.27	1366	0.96	-0.25
48b				1372	1.59	0.30	1368	1.72	0.39
48a				1374	17.21	-4.46	1368	20.08	-7.50
49a	1418	36.44	13.28	1414	14.70	7.16	1406	23.73	7.72
49b				1416	1.52	-0.06	1408	1.89	-0.07
50b	1432		-2.34	1422	1.04	0.92	1419	1.36	0.73
50a				1424	15.37	-13.55	1419	20.45	-12.14
51b	1442	119.54	-12.24	1433	2.17	-0.05	1430	1.56	0.07
51a				1433	21.07	3.18	1429	13.13	-2.29
52b				1436	0.29	0.35	1431	3.67	0.80
52a				1438	37.00	7.18	1432	82.16	7.63
53b				1437	1.51	0.56	1432	0.08	0.12
53a				1439	18.47	-17.01	1434	13.42	-12.69
54a				1445	8.43	0.53	1438	22.49	2.11
54b				1446	2.04	0.23	1441	2.29	-0.18
55a	1456	76.75		1449	30.75	-17.71	1444	56.70	14.51
55b				1451	1.42	0.86	1446	0.59	-0.03
56a				1449	22.97	4.81	1444	15.76	-26.60
56b				1453	1.02	0.12	1447	2.50	1.01
57a				1450	22.07	-4.59	1445	21.63	-3.08
57b				1459	1.42	-0.71	1453	1.42	-0.83
58b	1606	326.12	35.53	1601	17.54	-2.89	1590	31.21	-5.63
58a				1601	269.31	37.69	1592	572.02	92.12
59b	1674	522.48	-18.16	1681	22.93	-1.63	1654	30.44	0.97
59a				1681	374.56	10.34	1655	578.37	-32.76

Table S2: A quantitative comparison of the experimental and theoretical Rotational and Dipole strengths of each normal mode from 1000 cm^{-1} till 1800 cm^{-1}. D values in 10^{-40} esu^2 cm^2, R values in 10^{-44} esu^2 cm^2 and frequencies in cm^{-1}. The calculations of the 1:1 pulegone.$CDCl_3$ associations were compared to the experiment. The notations *a,b,c,…*refer to the different conformers, *a* being the most stable one.

	Experimental			B3LYP/3-311+G**		
Fund	Freq	D	R	Freq	D	R
43h	1013	14.13	23.33	988	0.760	0.677
43f				988	0.737	0.715
43g				988	0.736	0.715
43i				989	0.751	0.710
43e				989	0.803	0.752
43d				989	0.774	0.802
43j				989	1.005	0.552
43b				990	1.605	0.848
43a				990	1.616	0.857
43c				991	1.388	0.909
44j	1030	45.86		1006	5.413	0.003
44b				1007	7.068	0.251
44a				1007	7.005	0.287
44h				1007	5.935	0.410
44e				1008	6.072	0.406
44i				1008	5.920	0.402
44f				1008	5.955	0.312
44g				1008	5.950	0.318
44c				1008	7.149	0.206
44d				1008	6.286	0.362
45a	1063	29.94	-8.64	1055	2.755	-2.797
45b				1055	2.706	-2.751
45j				1056	1.950	-1.777
45c				1056	2.935	-2.829
45h				1056	1.236	-1.618
45f				1056	1.232	-1.592
45g				1056	1.228	-1.591
45i				1056	1.269	-1.659
45e				1057	1.320	-1.529
45d	1079		22.04	1057	1.527	-1.644
46j				1063	0.984	1.147
46h				1063	1.472	1.174
46a				1063	1.728	1.404
46b				1063	1.742	1.384
46c				1064	1.505	1.526
46f				1064	1.376	1.213
46g				1064	1.372	1.216
46i				1064	1.348	1.288
46e				1064	1.445	1.081
46d				1064	1.433	1.187
47j	1096	28.42	-5.55	1075	5.508	-0.990

47h				1075	5.566	-0.784
47a				1075	7.708	-0.617
47f				1075	5.687	-0.847
47g				1075	5.674	-0.843
47e				1075	5.804	-0.755
47b				1075	7.733	-0.631
47i				1075	5.493	-0.796
47c				1076	7.934	-0.778
47d				1076	6.140	-0.887
48h	1128	74.39	32.59	1100	6.424	1.213
48i				1101	6.575	1.252
48g				1101	6.622	1.240
48f				1101	6.627	1.242
48e				1101	6.878	1.261
48d				1102	7.358	1.299
48j				1103	3.332	1.272
48c				1105	3.966	1.992
48b				1105	5.050	2.234
48a				1106	4.951	2.250
49d				1106	5.922	1.009
49e				1106	5.787	0.976
49g				1106	6.069	0.958
49f				1106	6.071	0.957
49i				1106	6.031	1.004
49h				1106	6.267	0.956
49j				1109	7.877	0.982
49b				1110	11.101	1.196
49a				1110	11.167	1.216
49c				1110	11.835	1.270
50a	1140	42.49		1118	1.060	1.010
50b				1118	0.969	0.950
50j				1118	0.650	0.657
50c				1118	0.973	0.981
50e				1118	0.598	0.310
50d				1119	0.612	0.358
50i				1119	0.580	0.339
50g				1119	0.561	0.354
50f				1119	0.559	0.356
50h				1119	0.534	0.338
51j	1212	149.89	-48.19	1188	10.653	-2.902
51a				1189	16.785	-3.955
51b				1189	16.619	-4.014
51h				1189	10.604	-4.026
51c				1189	16.188	-4.073
51f				1189	10.656	-4.019
51g				1189	10.633	-4.021
51e				1189	11.144	-4.178
51d				1189	11.654	-4.321
51i				1190	10.531	-4.046
52f	1229		-19.44	1207	2.823	-1.067
52g				1207	2.836	-1.067
52h				1207	2.886	-1.028
52d				1208	2.853	-1.254

52i				1208	2.914	-1.030
52e				1208	2.713	-1.144
52j				1209	3.156	-1.242
52c				1211	4.827	-1.852
52a				1211	5.476	-1.902
52b				1211	5.634	-1.936
53g	1273	19.36	-10.13	1234	1.221	-0.407
53f				1234	1.220	-0.406
53i				1234	1.220	-0.414
53e				1234	1.363	-0.363
53j				1234	1.059	-0.697
53h				1234	1.126	-0.432
53d				1235	1.353	-0.335
53b				1236	2.075	-1.509
53a				1236	2.092	-1.545
53c				1236	1.798	-1.372
54h	1288	150.82	83.88	1258	8.787	4.432
54e				1258	8.654	4.636
54i				1258	8.594	4.409
54g				1259	8.834	4.425
54f				1259	8.846	4.431
54j				1259	9.979	4.451
54d				1259	9.493	4.898
54c				1260	15.779	6.895
54b				1261	14.161	6.506
54a				1261	14.180	6.583
55e				1266	2.788	1.873
55i				1266	2.606	1.718
55h				1266	2.395	1.611
55g				1266	2.564	1.725
55f				1266	2.567	1.727
55d				1267	2.862	1.933
55j				1268	1.708	0.989
55b				1271	2.994	1.603
55a				1271	3.003	1.615
55c				1272	1.665	1.010
56h				1295	0.173	0.358
56e				1295	0.179	0.119
56b				1295	0.455	0.645
56a				1295	0.461	0.668
56d				1295	0.201	0.111
56g				1295	0.189	0.263
56f				1295	0.189	0.261
56i				1295	0.172	0.258
56j				1296	0.263	0.409
56c				1296	0.404	0.595
57j	1336	24.74	-13.02	1316	1.381	0.964
57h				1316	1.482	1.230
57f				1316	1.335	1.139
57g				1316	1.341	1.144
57e				1316	1.296	1.072
57d				1316	1.323	1.067
57i				1316	1.453	1.193

57c				1318	1.492	1.257
57b				1319	1.322	1.288
57a				1319	1.371	1.297
58g				1322	1.879	-1.075
58f				1322	1.882	-1.074
58e				1323	1.937	-1.076
58i				1323	1.789	-1.098
58d				1323	2.076	-1.128
58h				1323	1.806	-1.111
58c				1324	2.056	-1.650
58b				1325	2.417	-1.603
58j				1325	1.502	-1.235
58a				1325	2.350	-1.629
59h	1373	132.11	-30.25	1349	1.331	-1.064
59f				1350	1.374	-0.932
59g				1350	1.373	-0.937
59i				1350	1.354	-1.026
59a				1350	2.071	-1.126
59b				1350	2.029	-1.113
59e				1350	1.355	-1.035
59d				1350	1.444	-0.970
59j				1350	1.565	-1.073
59c				1352	2.232	-0.731
60c	1385		-6.21	1361	3.748	-0.756
60j				1361	2.744	-0.231
60a				1361	4.174	-0.432
60b				1361	4.135	-0.454
60g				1362	2.112	-0.819
60f				1362	2.115	-0.830
60i				1363	2.088	-0.710
60h				1363	2.181	-0.509
60d				1363	2.060	-1.164
60e				1363	2.063	-0.918
61c				1365	1.181	0.679
61f				1365	1.259	0.665
61g				1365	1.257	0.658
61d				1365	1.679	1.067
61i				1365	1.298	0.617
61e				1365	1.592	0.926
61b				1366	1.003	0.450
61j				1366	0.914	0.341
61a				1366	0.988	0.462
61h				1366	1.190	0.443
62a				1370	2.294	-0.756
62b				1370	2.270	-0.751
62c				1371	2.096	-0.649
62j				1372	1.596	-0.764
62f				1374	1.733	-1.174
62g				1374	1.724	-1.173
62h				1375	1.537	-1.091
62i				1375	1.600	-1.207
62d				1375	1.861	-1.043
62e				1375	1.700	-1.051

63j	1418	36.44	13.28	1411	1.323	0.811
63c				1412	1.548	1.337
63a				1413	1.621	1.049
63h				1413	1.519	0.794
63b				1413	1.620	0.972
63f				1414	1.533	0.801
63g				1414	1.530	0.799
63i				1414	1.495	0.782
63d				1415	1.647	0.797
63e				1415	1.526	0.760
64a	1432		-2.34	1423	4.835	-2.831
64c				1423	4.282	-2.566
64b				1423	4.716	-2.742
64f				1423	1.488	-0.807
64g				1423	1.492	-0.803
64i				1423	1.572	-0.779
64e				1423	1.455	-0.941
64h				1423	1.533	-0.759
64d				1423	1.472	-0.982
64j				1424	2.083	-1.427
65c				1431	3.295	1.393
65a				1431	3.225	1.615
65b				1431	3.218	1.608
65j				1433	2.725	1.020
65h	1442	119.54	-12.24	1436	0.629	-0.517
65i				1436	0.904	-0.803
65g				1437	1.287	-0.843
65f				1437	1.294	-0.843
66a				1437	2.636	-2.549
66j				1437	1.970	-1.524
66c				1437	3.080	-2.516
65d				1437	1.040	-0.794
66b				1437	2.806	-2.633
65e				1437	1.385	-1.073
66f				1438	1.657	-1.570
66g				1438	1.641	-1.565
67j				1438	3.219	0.263
66e				1439	1.769	-1.480
66i				1439	1.703	-1.600
66d				1439	2.391	-1.707
67c				1439	4.335	0.280
66h				1439	1.122	-1.482
67b				1439	4.918	-0.140
67a				1439	5.342	-0.282
67h				1440	5.721	1.552
67i				1440	4.306	1.697
67f				1441	3.681	1.560
67g				1441	3.695	1.559
67d				1441	4.195	1.982
67e				1441	3.966	1.920
68h	1456	76.75		1445	1.301	0.010
68j				1446	0.484	-0.318
68i				1446	1.907	0.281

68f				1446	2.266	0.492
68g				1446	2.259	0.483
68c				1446	1.195	-0.417
68b				1446	1.108	-0.479
68a				1446	0.861	-0.470
68e				1446	1.978	0.530
68d				1446	1.975	0.493
69j				1447	3.090	-1.083
69c				1449	0.594	-0.950
69f				1449	1.795	-0.204
69e				1449	2.150	-0.225
69g				1449	1.784	-0.205
70c				1449	6.969	-0.399
69i				1449	1.580	-0.267
69d				1449	2.163	-0.278
69b				1449	3.075	-0.216
69a				1450	2.728	-0.206
69h				1449	3.504	-2.047
70j				1450	2.757	-0.240
71j				1450	1.064	0.042
70h				1450	1.582	0.989
70e				1450	1.758	-0.470
70b				1450	1.989	2.293
70a				1450	2.846	2.015
71h				1451	3.298	-0.448
70i				1451	1.890	-0.332
70f				1451	1.849	-0.450
70g				1451	1.847	-0.439
70d				1451	1.835	-0.555
71c				1451	1.750	-0.793
71b				1451	4.305	-3.895
71a				1451	3.761	-3.483
71i				1451	4.786	-0.764
71g				1451	4.649	-0.822
71f				1451	4.636	-0.820
71d				1452	4.968	-0.857
71e				1452	4.747	-0.839
72a	1606	326.12	35.53	1585	60.419	5.287
72b				1586	59.881	5.422
72c				1587	59.183	5.480
72j				1591	32.027	3.980
72e				1600	30.293	6.267
72d				1600	32.363	6.716
72i				1601	29.230	6.000
72f				1601	29.900	6.307
72g				1601	29.842	6.284
72h				1601	29.424	5.916
73c	1674	522.48	-18.16	1663	59.946	-0.241
73a				1663	62.545	-0.395
73b				1663	62.498	-0.292
73e				1667	49.499	0.455
73d				1668	52.501	0.725
73i				1669	50.072	0.722

73j		1669	48.399	0.862
73f		1669	50.778	0.867
73g		1669	50.761	0.865
73h		1670	51.395	0.910

Table S3 : A quantitative comparison of the experimental and theoretical Rotational and Dipole strengths of each normal mode from 1000 cm^{-1} till 1800 cm^{-1}. D values in 10^{-40} esu^2 cm^2, R values in 10^{-44} esu^2 cm^2 and frequencies in cm^{-1}. The PCM calculations of the 1:1 pulegone.$CDCl_3$ associations were compared to the experiment. The notations *a,b,c* refer to the different conformers, *a* being the most stable one.

	Experimental			B3LYP/3-311+G**		
fund	Freq	D	R	Freq	D	R
43a	1013	14.13	23.33	985	5.31	4.03
43b				987	4.82	3.95
43c				987	4.57	4.07
44a	1030	45.86		1006	32.10	1.86
44b				1007	31.39	1.28
44c				1007	30.85	1.04
45b	1063	29.94	-8.64	1054	6.93	-7.51
45a				1054	5.81	-6.78
45c				1055	7.33	-6.72
46a	1079		22.04	1062	9.99	4.92
46b				1062	9.04	5.49
46c				1062	9.01	5.14
47a	1096	28.42	-5.55	1073	25.63	-1.15
47c				1074	26.17	-2.29
47b				1074	26.13	-2.07
48a	1128	74.39	32.59	1099	50.78	4.67
48b				1100	47.83	5.06
48c				1100	48.05	4.71
49c				1103	22.96	5.02
49b				1104	25.39	4.67
49a				1104	23.87	4.98
50a	1140	42.49		1116	3.64	0.97
50c				1117	3.12	1.06
50b				1117	3.18	1.49
51b	1212	149.89	-48.19	1188	58.36	-16.10
51c				1188	57.94	-15.67
51a				1189	57.85	-16.77
52c	1229		-19.44	1205	10.00	-3.13
52b				1205	11.07	-3.05
52a				1205	11.14	-3.26
53a	1273	19.36	-10.13	1230	9.25	-1.73
53b				1230	8.56	-1.58
53c				1231	8.37	-1.34
54a	1288	150.82	83.88	1257	51.84	19.01
54b				1258	54.15	19.21

54c				1258	54.66	18.53
55a				1264	13.05	7.51
55b				1265	13.12	7.29
55c				1265	12.13	6.99
56a				1292	1.27	0.74
56b				1292	1.33	0.57
56c				1293	1.41	0.35
57a	1336	24.74	-13.02	1314	5.93	3.73
57c				1314	4.94	3.38
57b				1314	5.47	3.61
58b				1319	9.00	-4.35
58c				1319	9.75	-4.09
58a				1319	9.10	-4.30
59a	1373	132.11	-30.25	1347	6.04	-5.05
59b				1348	6.18	-4.33
59c				1348	5.82	-3.85
60b	1385		-6.21	1359	7.75	-4.76
60a				1359	8.78	-3.10
60c				1359	5.80	-5.13
61b				1361	6.15	4.03
61c				1362	8.19	4.43
61a				1362	5.21	2.74
62b				1369	8.16	-4.47
62c				1370	7.99	-3.67
62a				1371	7.81	-4.60
63c				1407	8.55	2.87
63b	1418	36.44	13.28	1407	8.64	3.01
63a				1408	8.56	3.07
64b	1432		-2.34	1420	8.54	-2.90
64c				1420	7.24	-3.04
64a				1420	8.87	-2.60
65a				1431	10.83	-3.36
65b	1442	119.54	-12.24	1431	13.53	-3.84
65c				1432	11.94	-4.18
66b				1434	4.92	-5.11
66c				1434	6.81	-5.85
66a				1434	6.55	-5.77
67c				1436	16.30	7.01
67b				1436	14.26	4.61
67a				1436	16.28	6.21
68a	1456	76.75		1440	16.58	1.52
68c				1440	14.86	2.48
68b				1440	18.43	2.38
69b				1443	7.72	-0.12
69c				1444	8.77	-0.36
69a				1444	8.51	-0.26
70c				1445	6.59	-2.02
70a				1445	7.85	-1.87
70b				1445	7.35	-1.98
71c				1447	21.83	-2.42
71b				1447	21.37	-2.29
71a				1448	22.45	-2.45
72b	1606	326.12	35.53	1588	218.40	42.07

72c				1590	218.23	41.77
72a				1591	218.46	42.59
73b	1674	522.48	-18.16	1649	236.23	-11.22
73c				1649	228.48	-12.45
73a				1649	236.24	-13.43

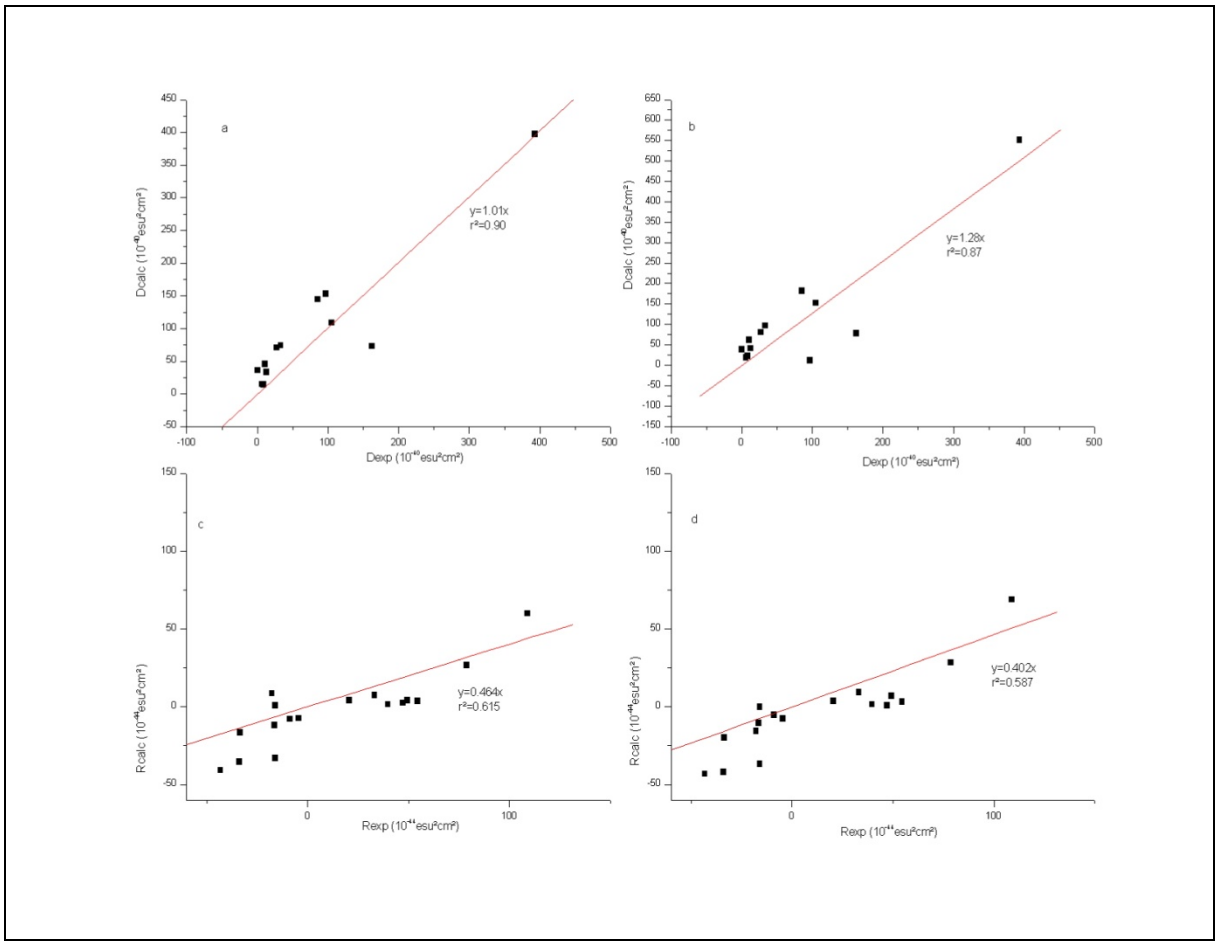

Figure S4: Comparison of the experimental Dipole strengths and the calculated ones: (a) calculations of pulegone in vacuum, (b) PCM calculations of pulegone in CS_2.Comparison of the experimental Rotational strengths and the calculated ones: (c) calculations of R - pulegone in vacuum, (d) PCM calculations of R – pulegone in CS_2.

Table S4: A quantitative comparison of the experimental and theoretical Rotational and Dipole strengths of each normal mode from 1000 cm^{-1} till 1800 cm^{-1}. D values in 10^{-40} esu² cm², R values in 10^{-44} esu² cm² and frequencies in cm^{-1}. The calculations of free pulegone in vacuum and the PCM calculations in CS_2 were compared with the experiment. The notations *a* and *b* refer to the different conformers, *a* being the most stable one.

	Experimental			B3LYP/6-311+G**			PCM		
Fund	Freq	D	R	Freq	D	R	Freq	D	R
22b	856		54.47	820	0.146	0.127	821	0.158	0.193
22a				837	3.913	3.532	837	4.526	3.088
23a	874		-16.06	859	31.983	-33.039	859	42.236	-36.639
23b	890		39.61	867	1.882	2.215	866	2.274	2.226
24b				886	0.269	-0.677	885	0.332	-0.564
24a	915		33.05	895	2.557	7.272	895	3.570	9.292
25b	933		-43.24	912	0.265	0.723	912	0.305	0.660
25a				916	19.497	-41.433	915	22.117	-43.754
26a	966		58.20	932	7.235	-14.465	930	14.821	-20.812
26b				935	0.090	0.450	935	0.225	1.001
27a				938	5.917	9.074	936	6.914	7.959
27b				941	0.262	0.758	940	0.213	0.407
28a				949	4.801	-24.452	947	4.535	-22.592
28b				955	0.619	2.204	953	0.630	2.103
29b	1013	6.01	49.26	971	0.916	-1.179	970	0.865	-1.129
29a				988	10.701	3.998	986	14.283	6.985
30b				988	2.815	1.347	988	3.329	1.247
30a	1028	33.18	47.06	1005	73.864	2.396	1004	97.162	0.810
31b	1078	10.32	47.30	1053	0.432	0.862	1051	0.881	1.026
31a				1056	17.217	-16.636	1055	20.383	-18.805
32b				1060	6.208	1.164	1058	7.441	1.113
32a				1062	21.186	7.732	1061	33.125	9.208
33b				1065	0.637	-0.758	1064	0.461	-0.822
33a	1095	27.43	-9.06	1073	70.589	-7.839	1072	80.510	-5.171
34b	1134	97.05	78.59	1086	7.756	1.211	1084	8.742	1.315
34a				1100	69.025	18.654	1099	113.624	18.463
35b				1102	3.212	-1.777	1101	4.198	-1.739
35a				1107	63.824	8.692	1106	69.287	10.265
36a	1170		20.56	1118	7.925	4.038	1117	9.820	3.475
36b				1122	1.385	0.045	1121	1.661	0.099
37b	1207	85.24	-33.95	1183	6.941	0.335	1182	7.642	-0.307
37a				1184	137.561	-35.731	1185	174.191	-41.705
38b	1250	0.00	-16.69	1194	0.225	-0.217	1193	0.640	0.156
38a				1209	36.046	-11.625	1207	38.242	-10.761
39b	1270	8.57	-4.53	1217	0.767	-0.579	1214	1.251	-0.597
39a				1234	13.108	-6.900	1231	21.061	-7.023
40a	1285	105.39	108.78	1256	84.085	51.074	1255	120.119	56.853
40b				1257	7.524	-1.942	1257	9.034	-2.178
41a				1265	17.322	10.345	1264	23.060	13.633
41b				1274	0.116	0.383	1272	0.222	0.467
42a	1337	12.78	-16.07	1295	2.385	3.815	1293	3.319	3.653
42b				1303	0.869	0.045	1301	0.885	0.050
43a				1317	14.107	9.389	1315	17.007	9.047
43b				1323	0.953	0.780	1320	18.599	-13.863
44a				1323	14.669	-13.610	1322	1.202	0.809
44b				1334	0.151	0.291	1333	0.153	0.331

45b	1371	162.44	-33.57	1340	0.103	-0.579	1339	0.082	-0.506
45a				1348	13.893	-10.640	1346	15.268	-12.607
46b				1362	1.874	0.270	1360	1.906	0.247
46a				1362	24.904	-6.996	1360	28.594	-6.771
47a				1366	12.080	5.690	1364	10.337	5.935
47b				1370	1.457	-0.274	1367	0.977	-0.281
48b				1372	1.594	0.296	1369	1.810	0.380
48a				1374	17.207	-4.460	1370	18.926	-6.366
59b	1680	393.42	-17.79	1681	22.926	-1.631	1662	28.384	-0.023
59a				1681	374.559	10.341	1663	523.277	-15.566

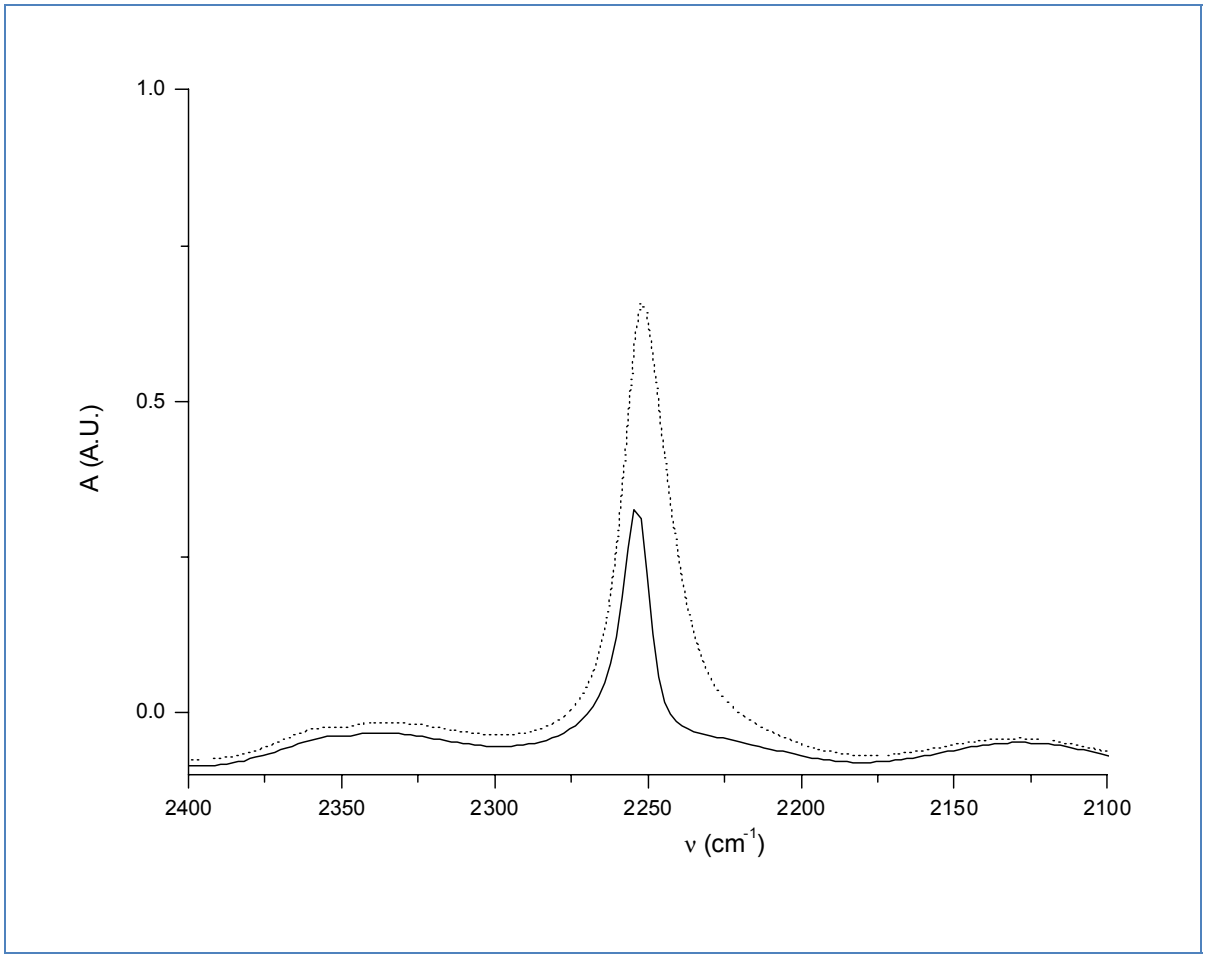

Figure S5: The IR – spectra of pure $CDCl_3$ (solid line) and of pulegone in $CDCl_3$, without solvent subtraction (dotted line).