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

Table S1. Equilibrium structural parameters of safrole conformers, computed at B2PLYP-D3/maug-cc-pVTZ level.

	SF1a	SF1b	SF2a	SF2b	SF3a	SF3b
C_1-C_2	1.404	1.404	1.401	1.4	1.403	1.402
C_2-C_3	1.392	1.392	1.395	1.395	1.393	1.393
C_3-C_4	1.407	1.407	1.405	1.404	1.406	1.406
C_4-C_5	1.374	1.374	1.377	1.377	1.375	1.375
C_1-C_6	1.374	1.374	1.376	1.376	1.375	1.375
C_1-H_7	1.079	1.079	1.079	1.079	1.079	1.079
C_2-H_8	1.081	1.081	1.081	1.081	1.081	1.081
C_4-H_9	1.08	1.08	1.08	1.08	1.08	1.08
C_3-C_{10}	1.514	1.513	1.515	1.515	1.505	1.505
C_{10}-H_{11}	1.092	1.092	1.092	1.092	1.093	1.093
C_{10}-H_{12}	1.092	1.092	1.092	1.092	1.093	1.093
C_{10}-C_{13}	1.5	1.501	1.5	1.5	1.508	1.507
C_{13}-H_{14}	1.085	1.085	1.085	1.085	1.085	1.085
C_{13}-C_{15}	1.33	1.33	1.33	1.33	1.33	1.33
C_{15}-H_{16}	1.08	1.08	1.08	1.08	1.08	1.08
C_{15}-H_{17}	1.082	1.082	1.082	1.082	1.081	1.081
C_5-O_{18}	1.375	1.375	1.375	1.375	1.375	1.375
C_6-O_{19}	1.375	1.375	1.376	1.376	1.376	1.376
O_{19}-C_{20}	1.43	1.43	1.43	1.43	1.43	1.43
C_{20}-H_{21}	1.094	1.094	1.094	1.085	1.094	1.085
C_{20}-H_{22}	1.085	1.085	1.085	1.094	1.085	1.094
C_1-C_2-C_3	122.2	122.2	122.1	122.1	122.2	122.2
C_2-C_3-C_4	119.9	119.9	119.8	119.9	119.8	119.8
C_3-C_4-C_5	117.4	117.4	117.5	117.5	117.5	117.5
C_2-C_1-C_6	116.7	116.7	116.8	116.8	116.7	116.7
C_6-C_1-H_7	121.6	121.6	121.5	121.5	121.5	121.5
C_1-C_2-H_8	118.8	118.8	119	119	118.9	118.9
C_3-C_4-H_9	121.2	121.2	121.4	121.4	121.3	121.3
C_2-C_3-C_{10}	120.8	120.9	120.2	120	120.5	120.5
C_3-C_{10}-H_{11}	108.5	108.5	110	110	109.6	109.6
C_3-C_{10}-H_{12}	110	110	108.5	108.6	109.8	109.7
C_3-C_{10}-C_{13}	112.5	112.5	112.9	112.6	114.8	114.8
C_{10}-C_{13}-H_{14}	115.9	115.9	115.9	115.9	114.9	115
C_{10}-C_{13}-C_{15}	124.7	124.7	124.7	124.7	126.1	126.1
C_{13}-C_{15}-H_{16}	121.6	121.6	121.6	121.6	120.9	120.9
C_{13}-C_{15}-H_{17}	121.3	121.3	121.3	121.3	121.8	121.7
C_4-C_5-O_{18}	128.3	128.3	128.3	128.3	128.4	128.4
C_1-C_6-O_{19}	128.8	128.8	128.8	128.8	128.8	128.8
C_6-O_{19}-C_{20}	104.6	104.6	104.5	104.5	104.6	104.5
O_{19}-C_{20}-H_{21}	109.2	109.2	109.3	109.5	109.2	109.5
O_{19}-C_{20}-H_{22}	109.5	109.5	109.5	109.3	109.5	109.2
C_4-C_3-C_{10}	119.3	119.2	119.9	120.1	119.6	119.6

C_1-C_2-C_3-C_4	0.3	0.2	0.4	0.4	0.1	0.1
C_2-C_3-C_4-C_5	-0.8	-0.1	-0.7	0.1	-0.5	0.2
C_6-C_1-C_2-C_3	0.3	-0.3	0.1	-0.6	0.2	-0.4
H_7-C_1-C_6-C_5	179.3	-179.6	179.3	-179.6	179.7	-179.3
C_6-C_1-C_2-H_8	-179.4	179.7	179.9	178.8	-179.7	179.3
C_2-C_3-C_4-H_9	178.6	179.5	179.3	-179.7	179.2	-179.9
C_1-C_2-C_3-C_{10}	-179.6	179.9	-178.9	-179.7	178.3	178
C_2-C_3-C_{10}-H_{11}	-0.7	1.8	70.1	64.2	28.4	29
C_2-C_3-C_{10}-H_{12}	116	118.5	-173.5	-179.2	143.8	144.5
C_2-C_3-C_{10}-C_{13}	-122.1	-119.6	-52.1	-57.8	-93.9	-93.2
C_3-C_{10}-C_{13}-H_{14}	59.3	59.2	-58.9	-58.7	-178.3	-178.4
C_3-C_{10}-C_{13}-C_{15}	-119.6	-119.8	120.2	120.4	1.9	1.8
C_{10}-C_{13}-C_{15}-H_{16}	179.5	179.5	-179.8	-179.7	179.8	179.8
C_{10}-C_{13}-C_{15}-H_{17}	-0.7	-0.7	0.4	0.5	-0.2	-0.2
C_3-C_4-C_5-O_{18}	177.8	-177.5	177.4	-177.6	178	-177.2
C_2-C_1-C_6-O_{19}	-177.4	177.6	-177.1	177.6	-177.8	177.1
C_1-C_6-O_{19}-C_{20}	-170.1	169.9	-170.1	169.8	-169.7	170.1
C_6-C_5-O_{18}-C_{20}	-10.5	10.4	-10.8	10.6	-10.4	10.8
C_6-O_{19}-C_{20}-H_{21}	98.1	-98.3	97.7	139.2	98.2	139.4
C_6-O_{19}-C_{20}-H_{22}	-139	138.9	-139.3	-97.9	-138.9	-97.7
C_4-C_3-C_{10}-C_{13}	58	60.1	128.6	122.1	84.3	84.7
H_{21}…H_{22}	1.806	1.805	1.806	1.806	1.806	1.806
C_{15}…C_1	5.945	5.933	5.125	5.136	4.59	4.579
C_{20}…C_{10}	5.97	5.97	5.977	5.978	5.966	5.963
C_{20}…C_{13}	6.534	6.453	6.932	6.814	6.717	6.615
C_{20}…C_{15}	7.228	7.16	8.032	7.943	6.476	6.283
C_2…C_{10}	2.528	2.528	2.524	2.521	2.517	2.517
C_2…C_{13}	3.601	3.583	3.026	3.063	3.41	3.405
C_2…C_{15}	4.804	4.792	3.773	3.797	3.606	3.597
C_3…C_{13}	2.507	2.506	2.512	2.509	2.538	2.538
C_3…C_{15}	3.566	3.566	3.575	3.572	2.937	2.937
C_4…C_{10}	2.521	2.52	2.529	2.53	2.516	2.516
C_4…C_{13}	3.056	3.071	3.651	3.606	3.325	3.328
C_4…C_{15}	3.773	3.785	4.843	4.813	3.485	3.49
C_4…C_{10}-C_{13}	95.5	96.3	128.2	125	108.8	109
C_4…C_{10}…C_{15}	95.5	97.7	148.1	145.7	87.3	87.5
A	2231.48	2208.9	3010.9	2912.18	2255.77	2213.1
B	551.24	552.56	490.41	493.27	573.8	577.4
C	457.31	459.12	434.23	438.89	519.59	523.52

Table S2. Equilibrium Cartesian coordinates of safrole conformers, computed at B2PLYP-D3/maug-cc-pVTZ level.

SF1a			
	X	Y	Z
C	-1.033578	1.818477	-0.153535
C	0.356213	1.795899	0.042564
C	1.054976	0.611609	0.261737
C	0.365818	-0.615344	0.285172
C	-0.995121	-0.579756	0.102225
C	-1.682543	0.608185	-0.112981
H	-1.566981	2.739815	-0.331185
H	0.899641	2.730424	0.027358
H	0.889400	-1.548921	0.430900
C	2.552785	0.623343	0.479403
H	2.903669	1.655050	0.415529
H	2.787622	0.269183	1.485507
C	3.286047	-0.219378	-0.522339
H	3.152886	0.057854	-1.562455
C	4.048013	-1.266386	-0.217247
H	4.548403	-1.843342	-0.981128
H	4.195628	-1.573979	0.809825
O	-1.874821	-1.634543	0.041721
O	-3.015267	0.337747	-0.318283
C	-3.170316	-1.028307	0.075962
H	-3.558335	-1.066836	1.097819
H	-3.824983	-1.534933	-0.625442

SF1b			
	X	Y	Z
C	1.027933	1.817784	0.168459
C	-0.364371	1.793802	-0.009577
C	-1.057851	0.615515	-0.272815
C	-0.360557	-0.603745	-0.362780
C	1.000899	-0.568320	-0.184139
C	1.682905	0.613598	0.076683
H	1.559438	2.736411	0.364845
H	-0.914503	2.721906	0.060080
H	-0.877855	-1.531673	-0.558592
C	-2.559803	0.623007	-0.457975
H	-2.913608	1.652692	-0.379350
H	-2.814726	0.273982	-1.460886
C	-3.267163	-0.229649	0.554218
H	-3.110647	0.040310	1.593017
C	-4.033144	-1.276571	0.259066
H	-4.513636	-1.860933	1.030061
H	-4.204013	-1.576855	-0.766547
O	1.899162	-1.605539	-0.269373
O	3.031385	0.357382	0.162262
C	3.123575	-1.067869	0.239318
H	3.239900	-1.365593	1.285256
H	3.950737	-1.410297	-0.373740

SF2a			
	X	Y	Z
C	0.465897	1.626294	-0.126641
C	-0.812949	1.069101	-0.253902
C	-1.024327	-0.309929	-0.250098
C	0.066030	-1.184028	-0.107084
C	1.318397	-0.625181	0.011358
C	1.516673	0.746959	0.001221
H	0.621381	2.694447	-0.122926
H	-1.663728	1.727981	-0.354648
H	-0.070895	-2.255575	-0.089826
C	-2.423451	-0.867388	-0.416349
H	-2.772498	-0.701815	-1.437956
H	-2.385242	-1.948655	-0.268872
C	-3.407654	-0.268931	0.543857
H	-3.179609	-0.395275	1.596645
C	-4.500419	0.401116	0.187809
H	-5.175158	0.814066	0.923349
H	-4.752483	0.552548	-0.853690
O	2.521206	-1.262044	0.207859
O	2.851455	1.020906	0.193112
C	3.504145	-0.239219	0.016985
H	3.895395	-0.303375	-1.002463
H	4.287501	-0.348013	0.759679

SF2b			
	X	Y	Z
C	0.481934	1.637630	-0.172898
C	-0.802811	1.096983	-0.308455
C	-1.029514	-0.279535	-0.329586
C	0.050773	-1.168255	-0.204371
C	1.308044	-0.625342	-0.062582
C	1.521415	0.744224	-0.047619
H	0.651328	2.703642	-0.166887
H	-1.647152	1.766964	-0.390256
H	-0.096228	-2.238415	-0.222928
C	-2.438467	-0.813725	-0.484910
H	-2.839844	-0.531074	-1.460177
H	-2.401700	-1.904696	-0.462443
C	-3.363202	-0.323431	0.589772
H	-3.076558	-0.564194	1.607735
C	-4.469130	0.383209	0.371881
H	-5.097139	0.715581	1.185468
H	-4.779233	0.647003	-0.630830
O	2.513806	-1.279785	0.030792
O	2.869822	0.999476	0.053261
C	3.447565	-0.260909	0.403534
H	4.372611	-0.400269	-0.146008
H	3.605258	-0.297169	1.485323

SF3a			
	X	Y	Z
C	0.616119	1.764116	0.177236
C	-0.711869	1.523465	-0.204429
C	-1.157148	0.259572	-0.585554
C	-0.262043	-0.825175	-0.591761
C	1.038711	-0.576987	-0.222302
C	1.470655	0.687325	0.154121
H	0.952768	2.745566	0.474460
H	-1.412734	2.346730	-0.202949
H	-0.585415	-1.817575	-0.870764
C	-2.599348	0.035085	-0.951610
H	-3.024793	0.959598	-1.349956
H	-2.665466	-0.691851	-1.765646
C	-3.472687	-0.441093	0.181143
H	-4.506604	-0.631076	-0.087127
C	-3.087596	-0.635150	1.439076
H	-3.788289	-0.976499	2.186827
H	-2.069539	-0.459206	1.755833
O	2.079625	-1.468729	-0.112848
O	2.797257	0.632283	0.513986
C	3.240274	-0.649950	0.060972
H	3.747649	-0.536759	-0.901328
H	3.886960	-1.094600	0.810193

SF3b			
	X	Y	Z
C	0.615494	1.765506	0.213812
C	-0.719858	1.534059	-0.146805
C	-1.165481	0.288161	-0.583234
C	-0.262920	-0.786736	-0.670501
C	1.042140	-0.550794	-0.308323
C	1.474124	0.695318	0.124873
H	0.955824	2.736567	0.539614
H	-1.427556	2.348674	-0.079326
H	-0.583153	-1.761834	-1.008062
C	-2.616040	0.069349	-0.917711
H	-3.058238	1.007375	-1.262691
H	-2.700445	-0.621767	-1.760804
C	-3.453911	-0.462427	0.216960
H	-4.494234	-0.646872	-0.029510
C	-3.031230	-0.709945	1.453281
H	-3.707843	-1.088755	2.205163
H	-2.005165	-0.541576	1.747592
O	2.110484	-1.415229	-0.355765
O	2.828668	0.655776	0.361616
C	3.154290	-0.736755	0.349661
H	4.095777	-0.883652	-0.169094
H	3.192151	-1.106950	1.378229

Table S3. Accuracy of equilibrium structures of SF conformers computed at different levels of theory [a,b] (distances in Å, angles in degrees, equilibrium rotational constants in %).

		SF1a	SF1b	SF2a	SF2b	SF3a	SF3b
				Bonds			
B3LYP[c]	MUE	0.005	0.005	0.005	0.005	0.005	0.005
	MAX	0.007	0.007	0.007	0.007	0.008	0.008
B3LYP-D3[c]	MUE	0.004	0.004	0.004	0.004	0.004	0.004
	MAX	0.006	0.006	0.006	0.006	0.006	0.006
B2PLYP[d]	MUE	0.001	0.001	0.001	0.001	0.001	0.001
	MAX	0.003	0.003	0.003	0.003	0.004	0.004
				Angles			
B3LYP	MUE	0.3	0.2	0.2	0.2	0.3	0.3
	MAX	1	1	0.9	1	1.2	1.2
B3LYP-D3	MUE	0.1	0.1	0.1	0.1	0.1	0.1
	MAX	0.6	0.6	0.6	0.6	0.6	0.6
B2PLYP	MUE	0.1	0.1	0.1	0.1	0.1	0.1
	MAX	0.4	0.4	0.2	0.3	0.4	0.5
				Distances			
B3LYP	MUE	0.035	0.036	0.037	0.038	0.044	0.045
	MAX	0.090	0.088	0.091	0.091	0.105	0.107
B3LYP-D3	MUE	0.015	0.015	0.015	0.021	0.014	0.014
	MAX	0.029	0.032	0.030	0.060	0.025	0.027
B2PLYP	MUE	0.014	0.014	0.013	0.013	0.016	0.017
	MAX	0.038	0.038	0.036	0.036	0.040	0.040
				Rotational Constants			
B3LYP	Ae	0.7	0.9	0.1	0.6	0.1	0.3
	Be	2.2	2.2	1.6	1.7	2.1	2.3
	Ce	1.7	1.8	1.4	1.6	2.1	2.3
B3LYP-D3	Ae	0.5	0.3	0.3	1.9	0.6	0.3
	Be	0.6	0.7	0.9	1.2	0.6	0.7
	Ce	0.8	0.9	0.9	1.5	0.7	0.8
B2PLYP	Ae	1.2	1.4	0.1	1	0.6	0.8
	Be	1.9	1.9	1.1	1.3	1.9	2
	Ce	1.3	1.4	0.9	1.2	1.8	2.1

[a] Mean Unsigned Error (MUE), Maximum Absolute Error (MAX) with respect to the B2PLYP-D3

[b] Mean relative absolute errors for rotational constants computed as $|B_e - B_e^{B2PLYP-D3}|*100/B_e^{B2PLYP-D3}$

[c] Computed with SNSD basis set.

[d] Computed with 6-311++G(2d,2p) basis set

Table S4. Harmonic vibrational frequencies and IR intensities of safrol conformers, computed at different level of theory: B2PLYP-D3, B2PLYP, B3LYP-D3 and B3LYP.

SF1a									
Mode	Approximate Description	B2PLYP-D3/maug		B2PLYP/6-311++G(2d,2p)		B3LYP-D3/SNSD		B3LYP/SNSD	
		v	I	v	I	v	I	v	I
1	τCC(R)CH$_2$+γC(R)-C+δCH$_2$	31	0	29	0	32	0	30	0
2	τCCC=C	73	0	73	0	72	0	72	0
3	τCOCC(OX)	108	3	107	3	101	5	101	5
4	τCOCC(OX)	150	7	150	8	134	4	132	4
5	τCCCC(R)+τCOCC(OX)+τCCC=C	211	0	209	0	210	0	210	0
6	τCOCC(OX)+δCCC+τCCCC(R)	255	1	254	1	250	1	250	1
7	δCCC+δCC=C+ τCOCC(OX)	288	2	288	2	287	2	285	2
8	τCOCC(OX)+δCCC(R)+τCCCC(R)	363	0	360	0	358	0	358	0
9	δCC=C+ τCCCC(R)	393	1	390	1	390	1	385	1
10	τCCCC(R)+δCCC(R)	430	6	429	6	429	6	429	6
11	δCCC(R)+τCCCC(R)+δCCC	455	3	453	3	453	3	451	3
12	δCCC(R)+δCC=C+δCH(R)	498	1	497	2	496	1	496	2
13	t=CH$_2$+γCH	603	7	600	7	601	8	599	7
14	τCCCC(R)+δCCC(R)+t=CH$_2$+γCH	619	7	615	7	617	7	617	7
15	t=CH$_2$+γCH+δCCC(R)+τCCCC(R)	678	10	675	10	676	9	673	9
16	δCOC+δCCC(R)	729	3	727	3	732	3	729	4
17	τCCCC(R)	742	0	738	1	740	1	740	1
18	νCC(R)+νCO +δCCC	792	17	788	18	788	16	787	16
19	τCCCC(R) +γCH	824	24	817	25	823	26	821	23
20	τCCCC(R) +γCH	835	18	828	15	832	15	831	17
21	γCH	887	13	876	14	883	12	882	12
22	r=CH$_2$+r-CH$_2$+ γCH	917	8	916	8	910	9	908	10
23	δCCC+ γCH+ ω=CH$_2$	939	2	929	1	937	24	935	20
24	γCH(R)+ ω=CH$_2$	949	32	943	37	939	15	940	13
25	νCO+ γCH+ ω=CH$_2$	954	46	947	50	947	18	945	17
26	ω=CH$_2$	956	4	953	1	951	14	948	16
27	γCH + r-CH$_2$+νCC+νCO	964	15	959	8	962	24	962	28
28	γCH + t=CH$_2$	1038	21	1033	22	1026	20	1026	21
29	νCO+δCH	1067	115	1060	115	1064	114	1062	113
30	δCH(R)+δCH+νCC(R)+ νCO	1114	15	1112	14	1109	14	1107	15
31	s-CH$_2$+δCH+νCC(R)	1130	6	1130	6	1123	6	1121	6
32	r-CH$_2$(OX)+δCH(R)	1143	8	1142	7	1137	8	1136	9
33	δCH(R)+r-CH$_2$(OX)	1157	10	1154	9	1143	14	1143	12
34	t–CH$_2$(OX)+δCH(R)+δCH+νCC(R)+ νCO	1207	23	1206	25	1199	18	1198	18
35	t–CH$_2$(OX)+ νCC(R)+ νCO	1235	16	1234	17	1220	17	1219	14
36	t–CH$_2$+ νCC(R)+ νCO	1240	2	1242	5	1230	2	1228	3
37	νCC(R)+t–CH$_2$	1283	252	1277	266	1279	253	1276	262
38	t–CH$_2$+δCH(R)	1296	28	1300	11	1287	30	1288	26
39	t-CH$_2$+νCC(R)+δCCH(R)	1324	3	1327	2	1316	3	1316	3
40	ω–CH$_2$+δCH+δCCH(R)	1335	2	1338	2	1328	2	1328	2
41	δCH +t–CH$_2$	1411	5	1403	10	1404	11	1399	12
42	ω–CH$_2$(OX)	1435	2	1435	2	1425	2	1425	2
43	s=CH$_2$+δCH+s-CH$_2$	1462	2	1466	6	1447	2	1447	2
44	s=CH$_2$+νCC(R)+δCCC(R)+t-CH$_2$+ ω–CH$_2$(OX)	1477	59	1472	59	1469	18	1466	22
45	s-CH$_2$	1492	33	1495	27	1477	75	1475	66
46	δCCH(R)+ νCC(R)+ s-CH$_2$(OX)	1525	192	1524	180	1523	180	1522	191
47	s-CH$_2$(OX)	1555	6	1554	4	1538	33	1538	26
48	νCC(R) + δCCC(R)	1653	5	1645	5	1653	5	1649	5
49	νCC(R) + δCCC(R)	1669	1	1662	1	1672	2	1669	1
50	νC=C + s=CH	1699	13	1693	13	1704	15	1700	15
51	ν $C_{20}H_{21}$	3026	116	3039	113	3003	128	3000	129
52	ν_s CH$_2$	3040	23	3047	23	3013	24	3010	24
53	ν_{as} CH$_2$	3081	11	3086	11	3053	12	3049	12
54	ν_{as} CH$_2$(OX)	3150	13	3152	12	3118	32	3113	33
55	νCH	3153	28	3162	5	3127	13	3125	14
56	ν_s =CH$_2$ +νCH	3159	4	3166	25	3136	5	3134	4
57	νCH(R)	3192	9	3195	8	3175	9	3172	9
58	νCH(R)	3212	1	3215	1	3198	2	3194	2
59	νCH(R)	3223	4	3226	4	3206	4	3204	4
60	ν_{as} =CH$_2$	3240	14	3244	13	3217	15	3215	15

SF1b

Mode	Approximate Description	B2PLYP-D3/Maug		B2PLYP/6-311++G(2d,2p)		B3LYP-D3/SNSD		B3LYP/SNSD	
		v	I	v	I	v	I	v	I
1	τCC(R)CH$_2$+γC(R)-C+δCH$_2$	30	0	30	0	30	0	28	0
2	τCCC=C	72	0	72	0	71	0	71	0
3	τCOCC(OX)	107	3	107	3	100	5	100	5
4	τCOCC(OX)	150	8	149	8	133	4	131	4
5	τCCCC(R)+τCOCC(OX)+τCCC=C	212	0	211	0	212	0	212	0
6	τCOCC(OX)+δCCC+τCCCC(R)	253	1	252	1	248	1	249	1
7	δCCC+δCC=C+ τCOCC(OX)	285	1	285	1	284	1	283	1
8	τCOCC(OX)+δCCC(R)+τCCCC(R)	369	1	367	1	363	1	362	1
9	δCC=C+ τCCCC(R)	391	1	389	1	389	1	385	1
10	τCCCC(R)+δCCC(R)	431	6	431	6	430	6	431	6
11	δCCC(R)+τCCCC(R)+δCCC	449	3	448	3	449	3	447	3
12	δCCC(R)+δCC=C+δCH(R)	498	2	497	2	496	1	495	2
13	t=CH$_2$+γCH	606	7	603	8	603	9	601	8
14	τCCCC(R)+δCCC(R)+ t=CH$_2$+γCH	616	7	612	6	614	6	614	6
15	t=CH$_2$+γCH+δCCC(R)+τCCCC(R)	681	9	678	9	678	8	675	8
16	δCOC+δCCC(R)	730	3	728	3	732	3	730	3
17	τCCCC(R)	741	1	736	1	739	1	739	1
18	νCC(R)+ νCO +δCCC	792	17	789	18	788	17	787	16
19	τCCCC(R) +γCH	825	28	819	31	824	30	823	26
20	τCCCC(R) +γCH	833	16	826	12	831	13	829	15
21	γCH	887	14	876	15	882	13	882	13
22	r=CH$_2$+r-CH$_2$+ γCH	916	5	916	5	909	7	907	7
23	δCCC+ γCH+ ω=CH$_2$	939	2	928	3	937	30	935	24
24	γCH(R)+ ω=CH$_2$	949	33	943	37	939	8	940	6
25	νCO+ γCH+ ω=CH$_2$	954	48	947	50	947	20	945	22
26	ω=CH$_2$	956	2	953	1	951	15	948	15
27	γCH + r-CH$_2$+νCC+νCO	965	14	959	8	963	23	963	27
28	γCH + t=CH$_2$	1037	20	1033	21	1026	20	1026	20
29	νCO+δCH	1067	113	1059	113	1064	112	1062	111
30	δCH(R)+δCH+νCC(R)+ νCO	1114	15	1112	15	1108	15	1106	16
31	s-CH$_2$+δCH+νCC(R)	1129	6	1129	6	1122	6	1120	6
32	r-CH$_2$(OX)+δCH(R)	1144	8	1142	7	1137	8	1136	8
33	δCH(R)+r-CH$_2$(OX)	1157	11	1154	10	1143	14	1143	13
34	t–CH$_2$(OX)+δCH(R)+δCH+νCC(R)+ νCO	1207	24	1206	25	1199	18	1198	18
35	t–CH$_2$(OX)+ νCC(R)+ νCO	1235	17	1233	18	1220	17	1219	15
36	t–CH$_2$+ νCC(R)+ νCO	1239	2	1241	6	1229	3	1227	3
37	νCC(R)+t–CH$_2$	1283	252	1277	265	1279	251	1276	261
38	t–CH$_2$+δCH(R)	1297	28	1301	11	1288	31	1288	27
39	ω–CH$_2$+δCH+δCCH(R)	1324	3	1327	2	1316	3	1316	3
40	δCH +t–CH$_2$	1335	2	1338	2	1328	1	1328	2
41	t-CH$_2$+νCC(R)+δCCH(R)	1411	5	1403	10	1404	11	1399	12
42	ω–CH$_2$(OX)	1435	2	1435	2	1425	2	1425	2
43	s=CH$_2$+δCH+s-CH$_2$	1462	2	1466	5	1447	2	1447	2
44	s=CH$_2$+νCC(R)+δCCC(R)+t-CH$_2$+ ω–CH$_2$(OX)	1477	61	1472	62	1469	19	1466	24
45	s-CH$_2$	1492	31	1495	26	1477	73	1475	64
46	δCCH(R)+ νCC(R)+ s-CH$_2$(OX)	1525	192	1524	181	1523	181	1522	193
47	s-CH$_2$(OX)	1555	6	1553	4	1538	32	1539	25
48	νCC(R) + δCCC(R)	1653	5	1645	5	1653	5	1649	5
49	νCC(R) + δCCC(R)	1669	1	1662	1	1672	2	1669	1
50	νC=C + s=CH	1698	13	1692	13	1704	16	1700	15
51	ν C$_{20}$H$_{21}$	3026	114	3039	112	3003	127	3001	127
52	ν$_s$ CH$_2$	3041	22	3047	21	3013	23	3010	22
53	ν$_{as}$ CH$_2$	3082	11	3087	11	3054	12	3049	12
54	ν$_{as}$ CH$_2$(OX)	3150	13	3152	13	3118	33	3113	34
55	νCH	3152	29	3162	5	3127	14	3125	15
56	ν$_s$ =CH$_2$ +νCH	3159	4	3165	26	3136	5	3134	4
57	νCH(R)	3192	9	3195	8	3175	9	3172	9
58	νCH(R)	3212	1	3215	1	3197	2	3194	2
59	νCH(R)	3223	4	3226	4	3206	4	3204	4
60	ν$_{as}$ =CH$_2$	3240	13	3244	13	3217	15	3215	15

		SF2a							
Mode	Approximate Description	B2PLYP-D3/Maug		B2PLYP/6-311++G(2d,2p)		B3LYP-D3/SNSD		B3LYP/SNSD	
		v	I	v	I	v	I	v	I
1	τCC(R)CH_2+γC(R)-C+δCH_2	20	0	19	0	22	0	19	0
2	τCCC=C	79	0	79	0	79	0	78	0
3	τCOCC(OX)	110	3	110	3	105	6	104	6
4	τCOCC(OX)	150	7	151	8	135	4	133	4
5	τCCCC(R)+τCOCC(OX)+τCCC=C	218	0	216	0	216	0	216	0
6	τCOCC(OX)+δCCC+τCCCC(R)	246	1	247	1	242	1	244	1
7	δCCC+δCC=C+ τCOCC(OX)	279	3	277	3	276	2	274	2
8	τCOCC(OX)+δCCC(R)+τCCCC(R)	356	0	354	0	352	0	351	0
9	δCC=C+ τCCCC(R)	390	1	388	1	387	1	384	1
10	τCCCC(R)+δCCC(R)	434	5	434	5	433	5	434	5
11	δCCC(R)+τCCCC(R)+δCCC	446	5	445	5	445	5	443	5
12	δCCC(R)+δCC=C+δCH(R)	509	4	508	4	508	4	507	4
13	t=CH_2+γCH	606	9	602	9	603	10	601	9
14	τCCCC(R)+δCCC(R)+ t=CH_2+γCH	612	6	609	6	611	5	610	6
15	t=CH_2+γCH+δCCC(R)+τCCCC(R)	684	9	681	9	681	8	678	8
16	δCOC+δCCC(R)	728	1	727	2	731	2	729	2
17	τCCCC(R)	744	1	740	1	741	1	741	1
18	νCC(R)+ νCO +δCCC	790	6	787	7	786	6	784	6
19	νCC(R)+ νCO	827	16	821	19	827	20	824	15
20	γCH+τCCCC(R)	835	24	828	19	831	18	831	22
21	γCH	878	13	869	14	874	12	875	12
22	r=CH_2+r-CH_2+ γCH	922	11	922	10	915	14	913	14
23	ω=CH_2+ω-CH_2+ γCH	928	15	926	16	922	13	919	13
24	νCO+ γCH+ ω=CH_2	951	8	940	2	939	37	940	37
25	γCH + ω=CH_2	953	31	945	37	950	1	949	1
26	ω=CH_2	956	53	949	50	955	49	954	47
27	νCC + νCO	975	8	971	8	971	9	968	11
28	γCH + t=CH_2	1037	19	1032	20	1025	20	1026	20
29	νCO+δCH	1067	128	1060	129	1064	126	1062	127
30	δCH(R)+δCH+νCC(R)+ νCO	1116	16	1113	15	1112	15	1109	16
31	s-CH_2+δCH+νCC(R)	1129	1	1130	1	1121	1	1119	0
32	r-CH_2(OX)+δCH(R)	1150	6	1149	5	1140	7	1140	6
33	δCH(R)+r-CH_2(OX)	1158	12	1155	11	1148	15	1146	14
34	t–CH_2(OX)+δCH(R)+δCH+νCC(R)+ νCO	1204	26	1204	27	1196	20	1195	19
35	t–CH_2(OX)+ νCC(R)+ νCO	1235	11	1234	13	1220	11	1219	9
36	t–CH_2+ νCC(R)+ νCO	1243	22	1244	29	1234	23	1231	22
37	νCC(R)+t–CH_2	1287	245	1281	250	1280	230	1279	247
38	t–CH_2+δCH(R)	1302	9	1305	5	1296	20	1295	11
39	ω–CH_2+δCH+δCCH(R)	1320	29	1325	19	1312	38	1312	35
40	δCH +t–CH_2	1333	6	1336	7	1327	8	1327	7
41	t-CH_2+νCC(R)+δCCH(R)	1403	3	1395	6	1396	7	1392	9
42	ω–CH_2(OX)	1434	2	1434	2	1424	2	1424	2
43	s=CH_2+δCH+s-CH_2	1462	1	1467	1	1448	1	1448	1
44	s=CH_2+νCC(R)+δCCC(R)+t-CH_2+ ω–CH_2(OX)	1479	58	1474	55	1472	27	1470	40
45	s-CH_2	1492	7	1495	8	1476	41	1474	24
46	δCCH(R)+ νCC(R)+ s-CH_2(OX)	1527	206	1526	197	1524	180	1523	195
47	s-CH_2(OX)	1554	8	1553	6	1538	49	1538	38
48	νCC(R) + δCCC(R)	1650	9	1643	9	1651	9	1647	9
49	νCC(R) + δCCC(R)	1668	0	1662	1	1671	0	1668	1
50	νC=C + s=CH_2	1699	14	1693	14	1704	17	1700	17
51	ν $C_{20}H_{21}$	3025	119	3038	115	3002	131	2999	132
52	ν_s CH_2	3039	23	3046	23	3011	25	3008	24
53	ν_{as} CH_2	3077	11	3083	10	3048	12	3045	12
54	ν_{as} CH_2(OX)	3150	13	3152	12	3119	33	3114	34
55	νCH	3153	28	3162	5	3127	13	3126	14
56	ν_s =CH_2 +νCH	3159	4	3166	26	3137	5	3134	4
57	νCH(R)	3198	3	3201	3	3183	3	3180	4
58	νCH(R)	3208	4	3212	4	3191	4	3188	4
59	νCH(R)	3223	3	3226	3	3206	4	3203	4
60	ν_{as} =CH_2	3241	14	3244	13	3217	15	3215	15

		SF2b							
Mode	Approximate Description	B2PLYP-D3/Maug		B2PLYP/6-311++G(2d,2p)		B3LYP-D3/SNSD		B3LYP/SNSD	
		v	I	v	I	v	I	v	I
1	τCC(R)CH$_2$+γC(R)-C+δCH$_2$	15	0	19	0	20	0	14	0
2	τCCC=C	78	0	78	0	78	0	77	0
3	τCOCC(OX)	110	3	107	3	103	6	103	6
4	τCOCC(OX)	150	8	150	9	134	4	132	4
5	τCCCC(R)+τCOCC(OX)+τCCC=C	216	0	213	0	213	0	214	0
6	τCOCC(OX)+δCCC+τCCCC(R)	253	1	253	1	245	0	248	0
7	δCCC+δCC=C+ τCOCC(OX)	271	0	269	0	273	0	268	0
8	τCOCC(OX)+δCCC(R)+τCCCC(R)	365	2	363	2	358	1	359	1
9	δCC=C+ τCCCC(R)	385	1	383	1	384	1	380	1
10	τCCCC(R)+δCCC(R)	434	5	432	5	432	5	433	5
11	δCCC(R)+τCCCC(R)+δCCC	447	5	446	5	446	5	444	5
12	δCCC(R)+δCC=C+δCH(R)	507	3	506	4	507	3	506	4
13	t=CH$_2$+γCH	606	5	604	6	605	13	602	10
14	τCCCC(R)+δCCC(R)+ t=CH$_2$+γCH	610	11	605	11	607	3	607	7
15	t=CH$_2$+γCH+δCCC(R)+τCCCC(R)	685	7	682	7	683	6	679	7
16	δCOC+δCCC(R)	729	1	728	1	732	1	729	1
17	τCCCC(R)	742	1	738	1	740	1	740	1
18	νCC(R)+ νCO +δCCC	790	8	787	9	786	7	785	8
19	νCC(R)+ νCO	827	17	822	24	828	24	825	16
20	γCH+τCCCC(R)	834	21	827	14	830	14	830	20
21	γCH	879	15	870	15	874	14	876	14
22	r=CH$_2$+r-CH$_2$+ γCH	922	8	922	10	914	12	912	11
23	ω=CH$_2$+ω-CH$_2$+ γCH	929	13	927	11	922	12	920	11
24	νCO+ γCH+ ω=CH$_2$	949	15	937	9	939	37	940	37
25	γCH + ω=CH$_2$	952	25	944	32	949	3	948	4
26	ω=CH$_2$	956	54	949	50	955	46	955	43
27	νCC + νCO	974	8	970	7	970	9	967	12
28	γCH + t=CH$_2$	1036	19	1031	20	1025	20	1025	20
29	νCO+δCH	1067	126	1059	126	1064	125	1062	126
30	δCH(R)+δCH+νCC(R)+ νCO	1117	17	1114	16	1112	16	1110	17
31	s-CH$_2$+δCH+νCC(R)	1126	1	1127	1	1120	1	1117	1
32	r-CH$_2$(OX)+δCH(R)	1150	5	1148	4	1140	6	1140	5
33	δCH(R)+r-CH$_2$(OX)	1158	13	1155	12	1148	16	1146	14
34	t–CH$_2$(OX)+δCH(R)+δCH+νCC(R)+ νCO	1205	28	1204	27	1197	20	1196	20
35	t–CH$_2$(OX)+ νCC(R)+ νCO	1235	12	1234	13	1219	11	1219	9
36	t–CH$_2$+ νCC(R)+ νCO	1241	22	1241	28	1233	23	1229	23
37	νCC(R)+t–CH$_2$	1288	246	1281	250	1281	230	1279	249
38	t–CH$_2$+δCH(R)	1303	5	1306	4	1296	18	1296	7
39	ω–CH$_2$+δCH+δCCH(R)	1320	29	1324	18	1313	39	1312	36
40	δCH +t–CH$_2$	1333	7	1336	8	1327	8	1327	7
41	t-CH$_2$+νCC(R)+δCCH(R)	1403	3	1395	6	1396	7	1391	9
42	ω–CH$_2$(OX)	1434	2	1434	2	1424	2	1424	2
43	s=CH$_2$+δCH+s-CH$_2$	1462	1	1467	1	1448	1	1448	1
44	s=CH$_2$+νCC(R)+δCCC(R)+t-CH$_2$+ ω–CH$_2$(OX)	1479	58	1474	56	1472	27	1469	41
45	s-CH$_2$	1493	6	1496	7	1477	40	1474	21
46	δCCH(R)+ νCC(R)+ s-CH$_2$(OX)	1528	205	1526	199	1525	182	1524	196
47	s-CH$_2$(OX)	1554	8	1553	6	1538	47	1539	36
48	νCC(R) + δCCC(R)	1650	9	1642	9	1650	9	1646	9
49	νCC(R) + δCCC(R)	1669	0	1662	1	1671	0	1668	1
50	νC=C + s=CH$_2$	1698	14	1692	14	1704	17	1700	17
51	ν $C_{20}H_{21}$	3025	117	3038	114	3002	130	2999	130
52	ν_s CH$_2$	3042	23	3048	22	3012	23	3010	23
53	ν_{as} CH$_2$	3081	10	3086	10	3050	12	3048	11
54	ν_{as} CH$_2$(OX)	3150	13	3152	13	3119	34	3114	34
55	νCH	3153	29	3162	5	3127	14	3126	14
56	ν_s =CH$_2$ +νCH	3159	4	3167	26	3136	5	3134	4
57	νCH(R)	3197	4	3199	5	3183	3	3178	4
58	νCH(R)	3208	4	3212	4	3192	4	3189	4
59	νCH(R)	3223	3	3226	3	3206	4	3203	4
60	ν_{as} =CH$_2$	3241	14	3244	13	3217	15	3215	15

		SF3a							
Mode	Approximate Description	B2PLYP-D3/Maug		B2PLYP/6-311++G(2d,2p)		B3LYP-D3/SNSD		B3LYP/SNSD	
		v	I	v	I	v	I	v	I
1	τCC(R)CH_2+γC(R)-C+δCH_2	38	0	37	0	36	0	36	0
2	τCCC=C	77	1	78	1	75	2	77	2
3	τCOCC(OX)	130	0	132	0	117	7	116	7
4	τCOCC(OX)	138	9	138	9	130	0	128	0
5	τCCCC(R)+τCOCC(OX)+τCCC=C	198	1	197	1	195	1	193	1
6	τCOCC(OX)+δCCC+τCCCC(R)	255	1	253	1	249	0	247	0
7	δCCC+δCC=C+ τCOCC(OX)	293	1	290	1	292	1	289	1
8	τCOCC(OX)+δCCC(R)+τCCCC(R)	354	1	352	1	349	0	346	0
9	δCC=C+ τCCCC(R)	413	1	412	1	412	1	409	1
10	τCCCC(R)+δCCC(R)	430	4	429	4	428	4	429	4
11	δCCC(R)+τCCCC(R)+δCCC	456	1	453	1	455	1	452	1
12	δCCC(R)+δCC=C+δCH(R)	560	4	558	4	558	4	557	3
13	t=CH_2+γCH	569	14	568	13	563	13	563	13
14	τCCCC(R)+δCCC(R)+ t=CH_2+γCH	615	3	612	4	615	3	612	3
15	ω=CH_2+γCH+δCCC(R)+τCCCC(R)	673	10	671	9	671	9	670	9
16	δCOC+δCCC(R)	728	2	726	2	730	2	728	2
17	τCCCC(R)	745	1	739	1	740	2	740	1
18	νCC(R)+ νCO +δCCC	778	9	775	10	776	9	774	9
19	νCC(R)+ νCO	825	19	820	20	826	21	823	17
20	τCCCC(R) +γCH	836	19	828	17	832	15	831	18
21	γCH	883	12	873	13	878	12	878	11
22	νCC+ νCO+ γCH	915	11	910	10	910	11	907	12
23	νCC+ νCO+ r–CH_2	942	8	931	1	934	15	932	14
24	γCH(R)	944	2	940	10	941	0	942	0
25	νCO+ γCH+ ω=CH_2	954	15	947	22	946	5	945	5
26	ω=CH_2	959	59	951	51	954	57	954	54
27	γCH + r-CH_2	976	3	973	2	969	7	968	11
28	γCH + t=CH_2	1040	14	1037	15	1027	14	1029	14
29	νCO+δCH	1067	119	1059	119	1064	117	1062	117
30	r=CH_2+δCH	1078	2	1080	2	1071	1	1070	2
31	δCH(R)+δCH+νCC(R)+ νCO	1122	16	1120	15	1117	16	1115	16
32	r-CH_2(OX)+δCH(R)	1146	7	1145	6	1139	8	1138	9
33	δCH(R)+r-CH_2(OX)	1158	9	1154	8	1145	10	1144	9
34	t–CH_2(OX)+δCH(R)+δCH+νCC(R)+ νCO	1207	5	1208	13	1197	3	1197	4
35	t–CH_2+ νCC(R)+ νCO	1215	33	1217	32	1205	26	1205	25
36	t–CH_2(OX)+ νCC(R)+ νCO	1236	20	1234	21	1221	25	1220	21
37	νCC(R)+t–CH_2	1287	250	1280	248	1281	251	1279	256
38	t–CH_2+δCH(R)	1305	10	1307	6	1298	12	1298	11
39	δCH +t–CH_2	1329	3	1334	3	1322	3	1322	2
40	ω–CH_2+δCH+δCCH(R)	1364	7	1367	4	1354	7	1355	7
41	t-CH_2+νCC(R)+δCCH(R)	1410	7	1401	12	1403	13	1398	15
42	ω–CH_2(OX)	1435	2	1434	2	1425	2	1425	2
43	s=CH_2+δCH+s-CH_2	1456	2	1461	2	1442	3	1442	2
44	s-CH_2	1480	83	1475	79	1472	19	1471	38
45	s=CH_2+νCC(R)+δCCC(R)+t-CH_2+ ω–CH_2(OX)	1492	10	1495	11	1476	79	1473	54
46	δCCH(R)+ νCC(R)+ s-CH_2(OX)	1528	173	1527	165	1526	148	1524	166
47	s-CH_2(OX)	1555	6	1553	5	1538	42	1539	31
48	νCC(R) + δCCC(R)	1652	6	1645	6	1653	6	1648	6
49	νCC(R) + δCCC(R)	1670	0	1663	0	1673	0	1670	0
50	νC=C + s=CH_2	1699	17	1694	17	1703	19	1702	20
51	ν $C_{20}H_{21}$	3026	118	3038	110	3003	130	3000	129
52	ν_s CH_2	3033	27	3039	31	3005	29	3002	30
53	ν_{as} CH_2	3062	11	3067	10	3034	12	3029	11
54	ν_{as} CH_2(OX)	3147	26	3150	26	3118	32	3113	33
55	νCH	3152	27	3166	25	3126	28	3122	29
56	ν_s =CH_2 +νCH	3166	8	3168	8	3145	8	3143	7
57	νCH(R)	3193	7	3196	7	3176	8	3173	8
58	νCH(R)	3209	2	3213	2	3194	3	3191	3
59	νCH(R)	3223	3	3226	3	3206	4	3204	4
60	ν_{as} =CH_2	3249	13	3252	13	3227	14	3225	14

				SF3b					
Mode	Approximate Description	B2PLYP-D3/Maug		B2PLYP/6-311++G(2d,2p)		B3LYP-D3/SNSD		B3LYP/SNSD	
		ν	I	ν	I	ν	I	ν	I
1	τCC(R)CH$_2$+γC(R)-C+δCH$_2$	38	0	37	0	37	0	37	0
2	τCCC=C	75	1	77	1	75	2	76	2
3	τCOCC(OX)	130	0	130	0	124	8	121	8
4	τCOCC(OX)	143	9	143	9	130	0	128	0
5	τCCCC(R)+τCOCC(OX)+τCCC=C	197	1	195	1	195	1	192	1
6	τCOCC(OX)+δCCC+τCCCC(R)	255	1	252	1	249	1	247	1
7	δCCC+δCC=C+ τCOCC(OX)	293	1	290	1	292	1	289	1
8	τCOCC(OX)+δCCC(R)+τCCCC(R)	356	0	353	0	350	0	347	0
9	δCC=C+ τCCCC(R)	415	2	414	2	414	2	411	2
10	τCCCC(R)+δCCC(R)	431	4	430	4	430	4	430	4
11	δCCC(R)+τCCCC(R)+δCCC	454	2	451	2	453	2	450	2
12	δCCC(R)+δCC=C+δCH(R)	559	5	557	5	557	5	556	5
13	t=CH$_2$+γCH	570	13	568	13	564	13	563	12
14	τCCCC(R)+δCCC(R)+ t=CH$_2$+γCH	611	2	608	2	611	2	609	2
15	ω=CH$_2$+γCH+δCCC(R)+τCCCC(R)	676	8	674	8	674	8	673	8
16	δCOC+δCCC(R)	729	1	727	1	730	2	728	2
17	τCCCC(R)	742	2	737	1	740	2	739	2
18	νCC(R)+ νCO +δCCC	779	10	776	12	776	11	774	11
19	νCC(R)+ νCO	827	21	821	24	827	25	824	19
20	τCCCC(R) +γCH	834	19	826	14	831	12	830	18
21	γCH	883	13	873	13	878	12	878	11
22	νCC+ νCO+ γCH	915	9	910	8	910	9	907	11
23	νCC+ νCO+ r–CH$_2$	941	13	931	4	934	18	932	16
24	γCH(R)	944	0	940	9	941	1	942	1
25	νCO+ γCH+ ω=CH$_2$	954	11	947	17	945	7	944	8
26	ω=CH$_2$	958	62	950	56	954	54	954	51
27	γCH + r-CH$_2$	976	3	973	3	969	7	968	11
28	γCH + t=CH$_2$	1040	14	1037	15	1027	13	1029	14
29	νCO+δCH	1067	115	1059	115	1064	114	1062	114
30	r=CH$_2$+δCH	1078	2	1080	2	1071	2	1070	2
31	δCH(R)+δCH+νCC(R)+ νCO	1122	15	1120	15	1117	15	1115	16
32	r-CH$_2$(OX)+δCH(R)	1147	3	1145	2	1139	3	1138	2
33	δCH(R)+r-CH$_2$(OX)	1158	12	1154	11	1146	14	1144	14
34	t–CH$_2$(OX)+δCH(R)+δCH+νCC(R)+ νCO	1207	5	1208	13	1197	3	1197	4
35	t–CH$_2$+ νCC(R)+ νCO	1215	33	1217	31	1205	26	1205	25
36	t–CH$_2$(OX)+ νCC(R)+ νCO	1236	20	1235	21	1222	24	1221	20
37	νCC(R)+t–CH$_2$	1286	249	1280	248	1281	250	1278	255
38	t–CH$_2$+δCH(R)	1305	10	1307	6	1298	11	1298	11
39	δCH +t–CH$_2$	1329	3	1334	3	1322	3	1322	2
40	ω–CH$_2$+δCH+δCCH(R)	1364	7	1367	4	1354	7	1355	7
41	t-CH$_2$+νCC(R)+δCCH(R)	1410	7	1401	12	1403	13	1398	15
42	ω–CH$_2$(OX)	1434	2	1434	2	1424	2	1424	2
43	s=CH$_2$+δCH+s-CH$_2$	1456	2	1461	2	1442	3	1442	2
44	s-CH$_2$	1480	83	1475	78	1472	19	1471	34
45	s=CH$_2$+νCC(R)+δCCC(R)+t-CH$_2$+ ω–CH$_2$(OX)	1491	10	1494	11	1476	79	1473	58
46	δCCH(R)+ νCC(R)+ s-CH$_2$(OX)	1528	172	1527	167	1526	145	1524	164
47	s-CH$_2$(OX)	1554	7	1553	5	1538	44	1538	33
48	νCC(R) + δCCC(R)	1652	6	1645	6	1653	6	1648	6
49	νCC(R) + δCCC(R)	1670	0	1663	0	1673	0	1670	0
50	νC=C + s=CH$_2$	1699	16	1694	17	1703	18	1702	19
51	ν C$_{20}$H$_{21}$	3025	113	3038	127	3002	129	2999	133
52	ν$_s$ CH$_2$	3033	25	3039	7	3005	22	3001	18
53	ν$_{as}$ CH$_2$	3062	11	3067	10	3034	12	3029	11
54	ν$_{as}$ CH$_2$(OX)	3148	26	3150	26	3120	34	3114	34
55	νCH	3153	28	3166	27	3126	28	3122	29
56	ν$_s$ =CH$_2$ +νCH	3166	8	3167	7	3144	8	3143	7
57	νCH(R)	3193	7	3195	7	3176	8	3173	8
58	νCH(R)	3209	2	3212	2	3194	3	3190	3
59	νCH(R)	3223	3	3226	3	3206	4	3204	4
60	ν$_{as}$ =CH$_2$	3249	13	3252	13	3227	14	3225	14

[a] Abbreviations: ν - bond stretching, δ - bending, deformation in plane, γ - out-of-plane bending, τ - torsion, s – scissoring, r – rocking, ω - wagging, t – twisting, R− phenolic ring, OX-1,3-dioxolane ring.

[b] The bands marked with an asterisk (*) are overlapped with the bands from the other conformers.

Table S5. Accuracy of harmonic and anharmonic fundamental vibrational wavenumbers and Zero Point Vibrational Energies of SF conformers computed at different levels of theory[a], all values in cm^{-1}.

		SF1a	SF1b	SF2a	SF2b	SF3a	SF3b
		Harmonic					
B3LYP[b]	MUE	10	10	10	10	10	10
	MAX	36	37	36	36	35	33
B3LYP-D3[b]	MUE	9	9	9	9	9	9
	MAX	31	32	31	31	30	28
B2PLYP[c]	MUE	4	4	4	4	4	4
	MAX	13	13	13	13	13	13
B2PLYP-D3d	ZPVE	39032	39029	39026	39022	39036	39037
B3LYP	ΔZPVE	-297	-297	-298	-297	-301	-299
B3LYP-D3	ΔZPVE	-248	-248	-247	-246	-253	-250
B2PLYP	ΔZPVE	-39	-38	-36	-37	-36	-41
		Anharmonic					
B2PLYP/B3e	MUE ALL	6	6	9	5	5	5
	MAX ALL	71	71	50	31	23	23
	MUE <2000	5	5	7	5	5	5
	MAX<2000	13	13	21	13	13	15
B2-D3/B3D3f	ZPVE	38578	38575	38590	38569	38593	38591
B2PLYP/B3e	ZPVE	38540	38537	38565	38535	38552	38539
B2PLYP/B3e	ΔZPVE	-37	-38	-25	-34	-41	-52

[a] Mean Unsigned Error (MUE) and Maximum Absolute Error (MAX), with respect to the B2PLYP-D3 (harmonic) and B2PLYP-D3/B3LYP-D3 (anharmonic) .

[b] Harmonic computations, SNSD basis set.

[c] Harmonic computations, 6-311++G(2d,2p) basis set

[d] Harmonic computations maug-cc-pVTZ basis set

[e] Hybrid model, harmonic part at B2PLYP/6-311++G(2d,2p) level and anharmonic corrections from B3LYP/SNSD computations.

[f] Hybrid model, harmonic part at B2PLYP-D3/maug-cc-pVTZ level and anharmonic corrections from B3LYP-D3/SNSD computations.

Table S6. Theoretical thermodynamic properties of SF conformers obtained within rigid-rotor harmonic-oscillator (RRHO) and hindered-rotor anharmonic oscillator (HRAO) models from hybrid B2PLYP/B3LYP and B2PLYP-D3/B3LYP-D3 computations.

			SF1a	SF1b	SF2a	SF2b	SF3a	SF3b
B2/B3	ΔH (kJ/mol)	RRHO	495.84	-0.01	0.02	-0.02	-0.08	-0.12
		HRAO[b]	491.15	0.02	-0.42	-0.42	0.17	0.03
	ΔS (J/mol· K)	RRHO	424.5	-0.04	2.53	2.75	-4.19	-4.22
		HRAO[b]	431.52	0.31	1.5	0.28	-3.76	-3.83
	ΔG (kJ/mol)	RRHO	369.3	0	-0.73	-0.84	1.17	1.14
		HRAO[b]	362.5	-0.07	-0.86	-0.5	1.29	1.17
B2D3/B3D3	ΔH (kJ/mol)	RRHO	496.21	-0.01	-0.01	-0.02	-0.09	-0.1
		HRAO[b]	491.42	-0.04	0.08	-0.5	0.27	0.27
	ΔS (J/mol· K)	RRHO	423.39	0.64	2.68	5.39	-3.61	-3.84
		HRAO[b]	430.03	0.56	2.11	1.52	-4.38	-3.59
	ΔG (kJ/mol)	RRHO	369.98	-0.2	-0.81	-1.63	0.99	1.04
		HRAO[b]	363.2	-0.21	-0.55	-0.95	1.57	1.34

[a] Values with respect to the SF1a conformer. All thermodynamic properties have been computed at 298 K and 1 atm.

[b] The two lowest vibrations have been described by hindered-rotor contributions computed by means of an automatic procedure[86] and anharmonic contributions from remaining modes computed by means of the HDCPT2 model using the hybrid force field in conjunction with simple perturbation theory (SPT)[38], (see text for details).

Table S7. Relative electronic energies [kJ/mol] of safrole conformers, computed at different levels of theory[a].

	B3LYP[b]	B3LYP-D3[b]	B3LYP-D3[c]	B2PLYP[d]	B2PLYP-D3[d]	B2PLYP-D3[e]	CCSD(T) [e]		
	SNSD	SNSD	SNSD	6-311++G(2d,2p)	6-311++G(2d,2p)	maug-cc-pVTZ	cc-pVTZ	cc-pVQZ	CBS+CV
SF1a	0	0	0	0	0	0	0	0	0.00 [a]
SF1b	0.04	0.06	0.06	0.19	0.19	0.06	0.06	0.06[f]	0.06 [f]
SF2a	1.24	1.25	1.27	1.36	1.39	1.37	1.44	1.37	1.33
SF2b	1.33	1.39	1.38	1.44	1.48	1.44	1.52	1.45 [f]	1.41 [f]
SF3a	2.64	0.22	0.09	1.76	0.43	0.62	0.6	0.52	0.42
SF3b	2.53	0.08	-0.06	1.63	0.28	0.45	0.44	0.36 [f]	0.26 [f]

[a] Energies relative to the SF1a conformer. The calculated absolute energy for SF1a is equal to -537.431160 (hartree) at CCSD(T)/CBS+CV level of theory.

[b] computed at B3LYP/SNSD optimized structure.

[c] computed at B3LYP-D3/SNSD optimized structure.

[d] computed at B2PLYP/6-311++G(2d,2p) optimized structure.

[e] computed at B2PLYP-D3/maug-cc-pVTZ optimized structure.

[f] difference between a and b conformers computed at the CCSD(T)/cc-pVTZ level.

Table S8. The best estimated vibrationally averaged rotational constants and dipole moment components (μ) .

	SF1a	SF1b	SF2a	SF2b	SF3a	SF3b
A_0/MHz	2223.48	2209.77	2977.97	2886.53	2248.40	2219.00
B_0/MHz	551.00	549.70	489.08	491.19	574.46	578.44
C_0/MHz	457.31	457.13	433.76	438.37	519.91	523.44
μ_a 298K/D	0.05	0.06	0.33	0.30	0.14	0.15
μ_b 298K/D	-0.19	0.03	-0.17	0.06	-0.40	-0.09
μ_c 298K/D	-0.28	-0.28	-0.28	-0.21	-0.09	-0.10
μ/D	0.53	0.41	0.56	0.45	0.72	0.27

Table S9. Selected structural and energetic parameters of transition states[a] .

Transition States	B2PLYP		B2PLYP-D3									
	ΔE	$\Delta E^{\#b}$	ΔE	ΔEZPVE	$\Delta E^{\#b}$	$\Delta EZPVE^{\#b}$	ΔG	$\Delta G^{\#b}$	ν	$C_2C_3C_{10}C_{13}$	$C_3C_{10}C_{13}C_{15}$	$C_6C_5O_{18}C_{20}$
tsSF1ab	2.08	2.08 / 2.03	2.11	3.37	2.11 / 2.05	3.37/3.31	1.71	1.71 / 1.85	115i	122.1	119.7	0.1
tsSF2ab	3.5	2.15 / 2.09	3.57	4.64	2.20 / 2.12	3.27/3.19	2.09	1.53 / 2.27	117i	-51.9	120.1	0.1
tsSF3ab	4.02	2.07 / 2.22	2.66	3.85	2.04 / 2.21	3.23/3.40	3.3	1.70 / 1.81	116i	-93.8	1.8	-0.2
tsSF(1-2)a	11.1	11.10 / 9.75	11.57	12.53	11.57 / 10.20	12.53/11.16	11.18	11.18 / 10.62	105i	-105.6	178.6	-12.8
tsSF(1-2)b	11	10.95 / 9.59	11.47	12.42	11.41 / 10.03	12.36/10.98	11.14	11.28 / 11.32	106i	-102.7	178.9	13
tsSF(1-3)a	14.33	14.33 / 12.38	13.67	15.16	13.67 / 13.05	15.16/14.54	14.75	14.75 / 13.14	130i	-83.9	-61.7	-12.8
tsSF(1-3)b	14.05	14.00 / 12.25	13.37	14.92	13.31 / 12.92	14.86/14.48	14.74	14.88 / 13.25	130i	-84.5	-61.6	13.3
tsSF(2-3)a	13.26	11.91 / 11.31	12.7	14.15	11.34 / 12.09	12.78/13.53	13.09	12.53 / 11.49	123i	-106.1	64	-12.8
tsSF(2-3)b	13.1	11.70 / 11.31	12.52	14.02	11.07 / 12.07	12.58/13.57	13.42	13.60 / 11.93	124i	-104	63.7	13.1

[a] Structures and frequencies B2PLYP-D3/SNSD, energies B2PLYP and B2PLYP-D3 with maug-cc-pVTZ basis set; ΔE, ZPVE corrected ΔEZPVE and ΔG at 298 K in kJ/mol are reported with respect to the SF1a conformer , wavenumber (ν) in cm^{-1}, angles in degrees.

[b] barriers to internal rotation are given for the direct/reverse reactionm with respect to the relevant mlocal minima.

Table S10. The Cartesian coordinates optimized structures of the SF transition states

	tsSF1ab		
	X	Y	Z
C	1.034977	1.828040	0.155405
C	-0.362492	1.806074	-0.024999
C	-1.063872	0.620841	-0.259183
C	-0.369163	-0.607805	-0.314419
C	0.997934	-0.572741	-0.140022
C	1.686677	0.614650	0.090304
H	1.572080	2.751945	0.337198
H	-0.909740	2.743270	0.016943
H	-0.893774	-1.543054	-0.479354
C	-2.567904	0.631558	-0.457280
H	-2.922934	1.665511	-0.368601
H	-2.815977	0.294100	-1.471668
C	-3.287243	-0.234592	0.540071
H	-3.140256	0.023396	1.588609
C	-4.054339	-1.283155	0.222946
H	-4.545140	-1.879032	0.985794
H	-4.215425	-1.572077	-0.812854
O	1.880601	-1.627253	-0.154460
O	3.030566	0.356283	0.231064
C	3.179658	-1.063462	0.081409
H	3.823909	-1.270359	-0.778039
H	3.592525	-1.482382	1.003751
	tsSF2ab		
	X	Y	Z
C	0.464488	1.632234	-0.141791
C	-0.820785	1.073090	-0.256875
C	-1.032412	-0.310338	-0.260004
C	0.064754	-1.187290	-0.136595
C	1.321812	-0.625885	-0.023277
C	1.519830	0.749011	-0.026278
H	0.621002	2.705007	-0.140474
H	-1.677095	1.735327	-0.339769
H	-0.070369	-2.263979	-0.132527
C	-2.436460	-0.869310	-0.411559
H	-2.799481	-0.699954	-1.433302
H	-2.395825	-1.956095	-0.267033
C	-3.412037	-0.273082	0.564433
H	-3.171374	-0.403554	1.619206
C	-4.513971	0.402436	0.221180
H	-5.183261	0.814805	0.969456
H	-4.778385	0.558451	-0.821869
O	2.528870	-1.272120	0.108336
O	2.861045	1.029673	0.103131
C	3.524192	-0.240005	0.193802
H	4.222837	-0.343329	-0.641512
H	4.036166	-0.312278	1.157877

tsSF3ab			
	X	Y	Z
C	0.614187	1.772889	0.191496
C	-0.722935	1.534107	-0.179454
C	-1.169851	0.272870	-0.583471
C	-0.265585	-0.809938	-0.629448
C	1.041947	-0.564472	-0.263666
C	1.474152	0.695107	0.137563
H	0.954004	2.754815	0.500496
H	-1.430530	2.357434	-0.147229
H	-0.587368	-1.799743	-0.936461
C	-2.619242	0.048970	-0.937108
H	-3.055002	0.984003	-1.313276
H	-2.692250	-0.665032	-1.768786
C	-3.477390	-0.454813	0.199827
H	-4.519411	-0.644169	-0.057879
C	-3.070403	-0.674628	1.454073
H	-3.761610	-1.035796	2.208670
H	-2.043000	-0.500064	1.758555
O	2.093825	-1.450166	-0.233225
O	2.816417	0.655687	0.437613
C	3.235570	-0.697145	0.204187
H	3.997470	-0.708818	-0.580794
H	3.613055	-1.124486	1.137609

tsSF12a			
	X	Y	Z
C	-0.890324	1.786976	-0.167801
C	0.478453	1.612912	0.116178
C	1.028219	0.359506	0.399234
C	0.200401	-0.784929	0.404398
C	-1.138860	-0.602574	0.129169
C	-1.674681	0.652837	-0.150519
H	-1.306707	2.762710	-0.390857
H	1.127078	2.483991	0.117846
H	0.601362	-1.771003	0.616696
C	2.506309	0.205172	0.670689
H	2.936660	1.187051	0.897240
H	2.649056	-0.408153	1.569495
C	3.263591	-0.424548	-0.484851
H	2.669287	-0.706826	-1.352465
C	4.582738	-0.642370	-0.498317
H	5.069973	-1.093769	-1.356315
H	5.214921	-0.375516	0.345478
O	-2.129896	-1.554828	0.036651
O	-3.018664	0.526614	-0.431046
C	-3.349290	-0.802095	-0.010303
H	-3.787216	-0.764149	0.995970
H	-4.025280	-1.253945	-0.735184

tsSF12b			
	X	Y	Z
C	0.881160	1.786074	0.176372
C	-0.490037	1.608367	-0.092423
C	-1.030945	0.361145	-0.417723
C	-0.191233	-0.772338	-0.484287
C	1.148486	-0.588567	-0.211641
C	1.675223	0.660254	0.111522
H	1.293655	2.759377	0.416649
H	-1.148878	2.470348	-0.042720
H	-0.582970	-1.750495	-0.744891
C	-2.513326	0.200077	-0.659189
H	-2.952048	1.179543	-0.880394
H	-2.671163	-0.417322	-1.552562
C	-3.244827	-0.427815	0.513939
H	-2.632543	-0.700528	1.372064
C	-4.561813	-0.655595	0.552839
H	-5.029818	-1.105640	1.422184
H	-5.211280	-0.398712	-0.280858
O	2.165885	-1.516002	-0.261091
O	3.040413	0.555018	0.273073
C	3.284291	-0.854607	0.344952
H	3.352440	-1.156356	1.398608
H	4.190346	-1.094325	-0.210109

tsSF13a			
	X	Y	Z
C	0.690142	1.773167	0.302592
C	-0.647666	1.587437	-0.089626
C	-1.129134	0.352780	-0.539879
C	-0.257009	-0.752509	-0.619834
C	1.055038	-0.558086	-0.234743
C	1.519892	0.673006	0.216802
H	1.053431	2.732223	0.654086
H	-1.328946	2.432082	-0.041104
H	-0.599697	-1.719186	-0.973846
C	-2.589775	0.189485	-0.905285
H	-2.941718	1.098615	-1.402185
H	-2.689753	-0.622635	-1.634758
C	-3.477659	-0.097980	0.294193
H	-4.248901	0.637249	0.516768
C	-3.368067	-1.173196	1.080982
H	-4.030306	-1.320528	1.927794
H	-2.607058	-1.931001	0.912125
O	2.076588	-1.481526	-0.185151
O	2.848894	0.562256	0.569327
C	3.258719	-0.697123	0.023937
H	3.753452	-0.528885	-0.941986
H	3.908759	-1.205674	0.734862

tsSF13b			
	X	Y	Z
C	0.697763	1.777084	0.330902
C	-0.649028	1.604117	-0.035438
C	-1.137333	0.390551	-0.533248
C	-0.263309	-0.704833	-0.691125
C	1.054668	-0.526884	-0.319100
C	1.526363	0.682921	0.181371
H	1.069934	2.724128	0.704958
H	-1.333340	2.440114	0.077448
H	-0.608586	-1.650049	-1.096886
C	-2.607734	0.235089	-0.859588
H	-2.982971	1.169512	-1.287670
H	-2.725515	-0.532084	-1.633815
C	-3.452927	-0.133933	0.348439
H	-4.223383	0.577829	0.639506
C	-3.307708	-1.252967	1.065288
H	-3.940816	-1.458216	1.922274
H	-2.545801	-1.990805	0.826568
O	2.100020	-1.418583	-0.424947
O	2.884453	0.590104	0.404352
C	3.161790	-0.812666	0.324444
H	3.173629	-1.236994	1.337351
H	4.105804	-0.966485	-0.196646

tsSF23a			
	X	Y	Z
C	0.651437	1.770342	-0.004946
C	-0.678665	1.477538	-0.366923
C	-1.117852	0.171479	-0.600245
C	-0.212581	-0.905797	-0.479687
C	1.087294	-0.607273	-0.130840
C	1.512626	0.699250	0.102985
H	0.981632	2.786375	0.179188
H	-1.383589	2.296805	-0.473428
H	-0.527374	-1.930680	-0.647587
C	-2.564209	-0.105161	-0.954102
H	-3.040628	0.834467	-1.254952
H	-2.607215	-0.768484	-1.824440
C	-3.349965	-0.727684	0.187243
H	-3.727789	-1.736869	0.033207
C	-3.593404	-0.117807	1.351658
H	-4.157095	-0.607948	2.138686
H	-3.225426	0.884816	1.556249
O	2.134521	-1.475586	0.086947
O	2.839456	0.690174	0.478339
C	3.291270	-0.632402	0.165183
H	3.794433	-0.620826	-0.810852
H	3.945529	-0.989276	0.959686

tsSF23b			
	X	Y	Z
C	0.642386	1.771658	-0.003003
C	-0.692684	1.477675	-0.344317
C	-1.124257	0.175775	-0.613485
C	-0.205507	-0.894975	-0.554476
C	1.096605	-0.596684	-0.213614
C	1.513957	0.705086	0.058200
H	0.970407	2.786035	0.193758
H	-1.409252	2.291862	-0.399932
H	-0.510813	-1.914423	-0.767173
C	-2.577831	-0.105246	-0.931177
H	-3.065898	0.833211	-1.216736
H	-2.639842	-0.766499	-1.801882
C	-3.331504	-0.734650	0.228089
H	-3.712230	-1.743403	0.078323
C	-3.543852	-0.132275	1.402469
H	-4.085707	-0.628028	2.201239
H	-3.171773	0.869553	1.603397
O	2.176750	-1.448714	-0.137581
O	2.869558	0.709232	0.310864
C	3.202466	-0.671677	0.494193
H	4.159394	-0.879977	0.017335
H	3.216573	-0.900612	1.568130

Table S11. Infrared frequencies and intensities of SF1, SF2 and SF3 in xenon matrices and their tentative assignment.

B2PLYP-D3/B3LYP-D3			Species	Xe(30K/11K)			Approximate Description[b]
ν_{anh} /cm^{-1}	I/km mol^{-1}	mode		ν/cm^{-1}	band	I[a]	
3106	17	60	SF3	3074		vw	ν_{as} =CH$_2$
3099	2	59	SF1	n.o.			νCH(R)
3098	18	60	SF1	3085		vw	ν_{as} =CH$_2$
3098	19	60	SF2	3063		vw	ν_{as} =CH$_2$
3094	5	59	SF2	n.o.			νCH(R)
3094	4	59	SF3	n.o.			νCH(R)
3072	3	57	SF2	n.o.			νCH(R)
3069	9	57	SF1	3080		vw	νCH(R)
3064	5	58	SF3	n.o.			νCH(R)
3063	5	58	SF2	3042		vw	νCH(R)
3063	3	58	SF1	n.o.			νCH(R)
3051	9	57	SF3	n.o.			νCH(R)
3026	9	56	SF3	n.o.			ν_s =CH$_2$+νCH
3023	6	56	SF1	3034		vw	ν_s =CH$_2$+νCH
3023	6	56	SF2	n.o.			ν_s =CH$_2$+νCH
3005	48	54	SF3	2979		sh,vw	ν_{as} CH$_2$(OX)
3002	30	55	SF3	n.o.			νCH
3002	45	54	SF2	2991		vw	ν_{as} CH$_2$(OX)
2999	14	55	SF1	2984		vw	νCH
2999	16	55	SF2	3009		vw	νCH
2988	43	54	SF1	2965		vw	ν_{as} CH$_2$(OX)
2968	68	45+47	SF3	2953		vvw	
2942	22	52	SF2	2968		sh,vw	ν_sCH$_2$
2938	14	53	SF1	2918		vvw	ν_{as}CH$_2$
2936	6	52	SF3	n.o.			ν_sCH$_2$
2933	13	53	SF2	2895		vw	ν_{as}CH$_2$
2918	12	53	SF3	2903		vvw	ν_{as}CH$_2$
2892	67	51	SF2	2879		sh,w	νC$_{20}$H$_{21}$
2891	93	51	SF1	2872		w	νC$_{20}$H$_{21}$
2890	58	51	SF3	2874		w	νC$_{20}$H$_{21}$
2871	24	52	SF1	2881		sh,vw	ν_sCH$_2$
2745-2780	2	over+combi	SF1	2773		vw	
2740-2790	2	over+combi	SF2	2768		vw	
1665	1	49	SF2	n.o.			νCC(R)+δCCC(R)
1660	2 (20)	50	SF1	1646		vw	νC=C+s=CH
1660	14	50	SF2	1645		sh,vw	νC=C+s=CH$_2$
1659	10	50	SF3	1639		vw	νC=C+s=CH$_2$
1635	1 (2)	49	SF1	n.o.			νCC(R)+δCCC(R)
1635	1 (3)	49	SF3	n.o.			νCC(R)+δCCC(R)
1620-1635	4	over+combi		1618		vw	
1614	2 (6)	48	SF1	1612		vw	νCC(R)+δCCC(R)
1610	4	48	SF3	1609		vw	νCC(R)+δCCC(R)
1609	6	48	SF2	1605		vw	νCC(R)+δCCC(R)
1519	9 (31)	47	SF2	1514		vw	s-CH$_2$(OX)
1516	25 (31)	47	SF1	1510		vw	s-CH$_2$(OX)
1516 (1510)	8 (47)	47	SF3	1507		sh, vw	s-CH$_2$(OX)
1493 (1496)	17 (145)	46	SF3	1502		sh, m	δCCH(R)+νCC(R)+s-CH$_2$(OX)
1494	160	46	SF2	1501		s	δCCH(R)+νCC(R)+s-CH$_2$(OX)
1493	75 (90)	46	SF1	1489		vs	δCCH(R)+νCC(R)+s-CH$_2$(OX)

1456	24 (52)	44	SF2	1445		sh, w	s=CH_2+νCC(R)+δCCC(R)+t-CH_2+ω–CH_2(OX)
1457 (1454)	8 (98)	44	SF1	1444		s	s=CH_2+νCC(R)+δCCC(R)+t-CH_2+ω–CH_2(OX)
1452	14	44	SF3	1447		sh, w	s-CH_2
1448	63 (85)	45	SF3	1447		sh, w	s=CH_2+νCC(R)+δCCC(R)+t-CH_2+ω–CH_2(OX)
1447	23	45	SF2	1430		sh, vw	s-CH_2
1443	10	45	SF1	1432		vw	s-CH_2
1429	1 (4)	43	SF1	n.o.			s=CH_2+δCH+s-CH_2
1429	1	43	SF2	n.o.			s=CH_2+δCH+s-CH_2
1421	3 (5)	43	SF3	1434		vw	s=CH_2+δCH+s-CH_2
1412	1	42	SF2	n.o.			ω–CH_2(OX)
1407 (1409)	1 (5)	42	SF3	1405		vvw	ω–CH_2(OX)
1406 (1398)	1 (4)	42	SF1	1409		vvw	ω–CH_2(OX)
1383	5	14+11	SF2	1397		vvw	
1380	8	41	SF1	1363		vw	δCH+t–CH_2
1379	7	41	SF3	1354		vw	t-CH_2+νCC(R)+δCCH(R)
1376 (1367)	2 (7)	41	SF2	1362		vw	t-CH_2+νCC(R)+δCCH(R)
1331	3	40	SF3	n.o.			ω–CH_2+δCH+δCCH(R)
1310	1 (13)	40	SF2	n.o.		vw	δCH+t-CH_2
1309	1	40	SF1	n.o.			ω–CH_2+δCH+δCCH(R)
1299 (1301)	1 (5)	39	SF1	1300		vw	t-CH_2+νCC(R)+δCCH(R)
1301	2	39	SF3	n.o.		vw	δCH+t-CH_2
1295	17 (24)	39	SF2	1287		vw	ω–CH_2+δCH+δCCH(R)
1282	11	38	SF3	1273		vw	t-CH_2+δCH(R)
1278	15	15+14	SF1	1268	A	vw	
1281 (1276)	5 (95)	38	SF2	1268	A	vw	t-CH_2+δCH(R)
1271	22 (44)	38	SF1	1248	B	w	t-CH_2+δCH(R)
1271	136	15+14	SF3	1254	B	sh, w	
1269	103	4+32	SF3	1249	B	vw	
1262	57	15+13	SF1	1235	C	sh,m	
1260	143	37	SF2	1236	C	m	νCC(R)+t-CH_2
1258	39 (48)	37	SF3	n.o.	C		νCC(R)+t-CH_2
1257	135 (156)	37	SF1	1231	C	sh, w	νCC(R)+t-CH_2
1249	12 (18)	32+3	SF3	n.o.	C		
1237	3	4+31	SF1	n.o.			
1212 (1225)	1 (17)	36	SF1	1224	D	w	t-CH_2+νCC(R)+νCO
1216	18 (31)	36	SF2	1221	D	w	t-CH_2+νCC(R)+νCO
1204	15 (18)	36	SF3	1196	E	vw	t-CH_2(OX)+νCC(R)+νCO
1203	4 (10)	35	SF2	1203	E	vw	t-CH_2(OX)+νCC(R)+νCO
1200	9	35	SF1	n.o.			t-CH_2(OX)+νCC(R)+νCO
1189	1 (17)	35	SF3	1183	F	vw	t-CH_2+νCC(R)+νCO
1184	9	34	SF2	1175	F	sh,vw	t-CH_2(OX)+δCH(R)+δCH+νCC(R)+νCO
1183	9 (20)	34	SF1	1174	F	vw	t-CH_2(OX)+δCH(R)+δCH+νCC(R)+νCO
1182	2	34	SF3	1178	F	vw	t-CH_2(OX)+δCH(R)+δCH+νCC(R)+νCO
1139	9	32	SF3	1127		vw	r-CH_2(OX)+δCH(R)
1137	7	32	SF2	1133	N	vw	r-CH_2(OX)+δCH(R)
1135	12	33	SF1	1132	N	vw	δCH(R)+r-CH_2(OX)
1131	17	33	SF2	1130	N	vw	δCH(R)+r-CH_2(OX)
1127	6	33	SF3	1122		vw	δCH(R)+r-CH_2(OX)
1126	10	32	SF1	1120	O	vw	r-CH_2(OX)+δCH(R)
1111	3 (6)	31	SF1	1117	P	vw	s-CH_2+δCH+νCC(R)
1107	2	31	SF2	1113	P	vw	s-CH_2+δCH+νCC(R)
1100	1	12+14	SF1	1098	Q	vw	
1105	9	31	SF3	1101		vw	δCH(R)+δCH+νCC(R)+νCO
1099	8	30	SF2	1091	Q	vw	δCH(R)+δCH+νCC(R)+νCO
1097	8 (12)	30	SF1	1089	Q	vw	δCH(R)+δCH+νCC(R)+νCO
1095	3	7+19	SF1	1094	Q	vw	

1061	1	30	SF3	n.o.			r=CH_2+δCH
1043 (1048)	48 (134)	29	SF2	1044		vs	νCO+δCH
1044	113	29	SF1	1044		vs	νCO+δCH
1043	96	29	SF3	1044		vs	νCO+δCH
1015	17	28	SF2	1024		vw	γCH+t=CH_2
1015	18	28	SF1	998		vw	γCH+t=CH_2
1016	10	28	SF3	993		vw	γCH+t=CH_2
1005	3	2+26	SF2	1000			
		3 quanta?	SF3	991		vw	
		3 quanta?	SF1	991		vw	
956	4 (16)	27	SF2	961		vw	νCC+νCO
956	3	7 +15	SF1	n.o.			
953	3	27	SF3	952	G	vw	γCH+r-CH_2
951	10	8+13	SF1	n.o.			
946	2(4)	11+12	SF2	946	H	sh, vw	
942	3 (37)	25	SF3	938	H	vw	νCO+γCH+ω=CH_2
941	5	11+12	SF1	n.o.			
939	10 (49)	26	SF1	944	H	w	νCO+γCH+ω=CH_2
938(939)	19 (49)	25	SF1	944	H	w	ω=CH_2
936	37 (87)	24	SF2	946	H	w	νCO+γCH+ω=CH_2
935	13	5+17	SF3	928	I	vw	
933	9	27	SF1	925	I	vw	γCH+r-CH_2+νCC+νCO
930	12	23	SF1	915	J	m	δCCC+γCH+ω=CH_2
927(926)	54 (87)	26	SF2	915	J	sh, m	ω=CH_2
927	9 (46)	23	SF3	911	J	vw	νCC+νCO+r-CH_2
926(927)	37 (46)	26	SF3	911	J	vw	ω=CH_2
925(926)	2 (87)	25	SF2	915	J	sh, m	γCH(R)+ω=CH_2
918	1	24	SF3	908	K	vw	γCH(R)
916	9	24	SF1	907	K	w	γCH(R)+ω=CH_2
914	6	23	SF2	906	K	vw	ω=CH_2+ω-CH_2+γCH
909	10	22	SF2	902	L	vw	r=CH_2+r-CH_2+γCH
907	8	22	SF1	903	L	vw	r=CH_2+r-CH_2+γCH
900	1	22	SF3	900	L	vw	νCC+νCO+γCH
879	10	3+18	SF3	868	M	vw	
869	11	21	SF3	856	M	vw	γCH
869	12	21	SF1	847	M	vw	γCH
858	10	21	SF2	848	M	vw	γCH
822	10	20	SF1	809	R	vw	τCCCC(R)+γCH
821	14	19	SF2	810	R	sh, vw	νCC(R)+νCO
820	16	19	SF3	817		vw	νCC(R)+νCO
814	1	5+14	SF1	800	S	vw	
812	12	20	SF2	804	S	vw	τCCCC(R)+γCH
811	12	20	SF3	776		vw	τCCCC(R)+γCH
807	3	4+15	SF2	801	T	sh, vw	
807	21	19	SF1	797	T	w	τCCCC(R)+γCH
781	8(17)	18	SF1	776		vw	νCC(R)+νCO+δCCC
780	3	18	SF2	776		vw	νCC(R)+νCO+δCCC
769	10	18	SF3	772		vw	νCC(R)+νCO+δCCC
744	1	17	SF3	765		vw	τCCCC(R)
740	1	17	SF2	n.o.			τCCCC(R)
729	0	17	SF1	n.o.			τCCCC(R)
720	4	16	SF1	721		vw	δCOC+δCCC(R)
719	3	16	SF3	726		vw	δCOC+δCCC(R)
719	4	16	SF2	717		vw	δCOC+δCCC(R)
675	8	15	SF2	667		vw	t=CH_2+γCH+δCCC(R)+τCCCC(R)
670	7(8)	15	SF1	666		vw	t=CH_2+γCH+δCCC(R)+τCCCC(R)
664	8	15	SF3	660		vw	ω=CH_2+γCH+δCCC(R)+τCCCC(R)
610	6	14	SF1	n.o.			τCCCC(R)+δCCC(R)+t=CH_2+γCH
609	3	14	SF3	n.o.			τCCCC(R)+δCCC(R)+t=CH_2+γCH
604	6	14	SF2	598		vw	τCCCC(R)+δCCC(R)+t=CH_2+γCH
599	12	13	SF2	585		vw	t=CH_2+γCH
594	8	13	SF1	584		sh, vw	t=CH_2+γCH
564	11	13	SF3	554		vw	t=CH_2+γCH

[a] Intensity: vs-very strong, s-strong, m-medium, w-weak, vw-very weak, sh-shoulder

[b]Abbreviations: ν - bond stretching, δ - bending, deformation in plane, γ - out-of-plane bending, τ - torsion, s – scissoring, r – rocking, ω - wagging, t – twisting, R− phenolic ring, OX-1,3-dioxolane ring.