1		U	1			
	SF1a	SF1b	SF2a	SF2b	SF3a	SF3b
C <sub>1</sub> -C <sub>2</sub>	1.404	1.404	1.401	1.4	1.403	1.402
C <sub>2</sub> -C <sub>3</sub>	1.392	1.392	1.395	1.395	1.393	1.393
C <sub>3</sub> -C <sub>4</sub>	1.407	1.407	1.405	1.404	1.406	1.406
C <sub>4</sub> -C <sub>5</sub>	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 <sub>1</sub> -H <sub>7</sub>	1.079	1.079	1.079	1.079	1.079	1.079
C <sub>2</sub> -H <sub>8</sub>	1.081	1.081	1.081	1.081	1.081	1.081
C <sub>4</sub> -H <sub>9</sub>	1.08	1.08	1.08	1.08	1.08	1.08
C <sub>3</sub> -C <sub>10</sub>	1.514	1.513	1.515	1.515	1.505	1.505
C <sub>10</sub> -H <sub>11</sub>	1.092	1.092	1.092	1.092	1.093	1.093
C <sub>10</sub> -H <sub>12</sub>	1.092	1.092	1.092	1.092	1.093	1.093
C <sub>10</sub> -C <sub>13</sub>	1.5	1.501	1.5	1.5	1.508	1.507
C <sub>13</sub> -H <sub>14</sub>	1.085	1.085	1.085	1.085	1.085	1.085
C <sub>13</sub> -C <sub>15</sub>	1.33	1.33	1.33	1.33	1.33	1.33
C <sub>15</sub> -H <sub>16</sub>	1.08	1.08	1.08	1.08	1.08	1.08
C <sub>15</sub> -H <sub>17</sub>	1.082	1.082	1.082	1.082	1.081	1.081
C <sub>5</sub> -O <sub>18</sub>	1.375	1.375	1.375	1.375	1.375	1.375
C <sub>6</sub> -O <sub>19</sub>	1.375	1.375	1.376	1.376	1.376	1.376
O <sub>19</sub> -C <sub>20</sub>	1.43	1.43	1.43	1.43	1.43	1.43
C <sub>20</sub> -H <sub>21</sub>	1.094	1.094	1.094	1.085	1.094	1.085
C <sub>20</sub> -H <sub>22</sub>	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 <sub>13</sub> -C <sub>15</sub> -H <sub>16</sub>	121.6	121.6	121.6	121.6	120.9	120.9
C <sub>13</sub> -C <sub>15</sub> -H <sub>17</sub>	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 <sub>1</sub> -C <sub>6</sub> -O <sub>19</sub>	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 <sub>19</sub> -C <sub>20</sub> -H <sub>22</sub>	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

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

$C_1 - C_2 - C_3 - C_4$	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
$H_{21} \ldots H_{22}$	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
$C_{20} \ldots C_{10}$	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
$C_2C_{10}$	2.528	2.528	2.524	2.521	2.517	2.517
$C_2C_{13}$	3.601	3.583	3.026	3.063	3.41	3.405
$C_2C_{15}$	4.804	4.792	3.773	3.797	3.606	3.597
$C_3C_{13}$	2.507	2.506	2.512	2.509	2.538	2.538
$C_3C_{15}$	3.566	3.566	3.575	3.572	2.937	2.937
$C_4C_{10}$	2.521	2.52	2.529	2.53	2.516	2.516
$C_4C_{13}$	3.056	3.071	3.651	3.606	3.325	3.328
$C_4C_{15}$	3.773	3.785	4.843	4.813	3.485	3.49
$C_4C_{10}$ - $C_{13}$	95.5	96.3	128.2	125	108.8	109
$C_4C_{10}C_{15}$	95.5	97.7	148.1	145.7	87.3	87.5
А	2231.48	2208.9	3010.9	2912.18	2255.77	2213.1
В	551.24	552.56	490.41	493.27	573.8	577.4
С	457.31	459.12	434.23	438.89	519.59	523.52

	Х	Y	Z
С	-1.033578	1.818477	-0.153535
С	0.356213	1.795899	0.042564
С	1.054976	0.611609	0.261737
С	0.365818	-0.615344	0.285172
С	-0.995121	-0.579756	0.102225
С	-1.682543	0.608185	-0.112981
Н	-1.566981	2.739815	-0.331185
Н	0.899641	2.730424	0.027358
Н	0.889400	-1.548921	0.430900
С	2.552785	0.623343	0.479403
Н	2.903669	1.655050	0.415529
Н	2.787622	0.269183	1.485507
С	3.286047	-0.219378	-0.522339
Н	3.152886	0.057854	-1.562455
С	4.048013	-1.266386	-0.217247
Н	4.548403	-1.843342	-0.981128
Н	4.195628	-1.573979	0.809825
0	-1.874821	-1.634543	0.041721
0	-3.015267	0.337747	-0.318283
С	-3.170316	-1.028307	0.075962
Н	-3.558335	-1.066836	1.097819
Н	-3.824983	-1.534933	-0.625442
		SF1b	
	Х	Y	Z
С	1.027933	1.817784	0.168459
С	-0.364371	1.793802	-0.009577
С	1.055051		
С	-1.05/851	0.615515	-0.272815
•	-1.057851 -0.360557	0.615515 -0.603745	-0.272815 -0.362780
C	-1.057851 -0.360557 1.000899	0.615515 -0.603745 -0.568320	-0.272815 -0.362780 -0.184139
C C	-1.057851 -0.360557 1.000899 1.682905	0.615515 -0.603745 -0.568320 0.613598	-0.272815 -0.362780 -0.184139 0.076683
C C H	-1.057851 -0.360557 1.000899 1.682905 1.559438	0.615515 -0.603745 -0.568320 0.613598 2.736411	-0.272815 -0.362780 -0.184139 0.076683 0.364845
C C H H	-1.057851 -0.360557 1.000899 1.682905 1.559438 -0.914503	0.615515 -0.603745 -0.568320 0.613598 2.736411 2.721906	-0.272815 -0.362780 -0.184139 0.076683 0.364845 0.060080
С С Н Н	-1.057851 -0.360557 1.000899 1.682905 1.559438 -0.914503 -0.877855	0.615515 -0.603745 -0.568320 0.613598 2.736411 2.721906 -1.531673	-0.272815 -0.362780 -0.184139 0.076683 0.364845 0.060080 -0.558592
С С Н Н С	-1.057851 -0.360557 1.000899 1.682905 1.559438 -0.914503 -0.877855 -2.559803	0.615515 -0.603745 -0.568320 0.613598 2.736411 2.721906 -1.531673 0.623007	-0.272815 -0.362780 -0.184139 0.076683 0.364845 0.060080 -0.558592 -0.457975
С С Н Н С Н	-1.057851 -0.360557 1.000899 1.682905 1.559438 -0.914503 -0.877855 -2.559803 -2.913608	0.615515 -0.603745 -0.568320 0.613598 2.736411 2.721906 -1.531673 0.623007 1.652692	-0.272815 -0.362780 -0.184139 0.076683 0.364845 0.060080 -0.558592 -0.457975 -0.379350
С С Н Н С Н Н	-1.057851 -0.360557 1.000899 1.682905 1.559438 -0.914503 -0.877855 -2.559803 -2.913608 -2.814726	0.615515 -0.603745 -0.568320 0.613598 2.736411 2.721906 -1.531673 0.623007 1.652692 0.273982	-0.272815 -0.362780 -0.184139 0.076683 0.364845 0.060080 -0.558592 -0.457975 -0.379350 -1.460886
С С Н Н С Н Н С	-1.057851 -0.360557 1.000899 1.682905 1.559438 -0.914503 -0.877855 -2.559803 -2.913608 -2.814726 -3.267163	0.615515 -0.603745 -0.568320 0.613598 2.736411 2.721906 -1.531673 0.623007 1.652692 0.273982 -0.229649	-0.272815 -0.362780 -0.184139 0.076683 0.364845 0.060080 -0.558592 -0.457975 -0.379350 -1.460886 0.554218
С С Н Н С Н С Н	-1.057851 -0.360557 1.000899 1.682905 1.559438 -0.914503 -0.877855 -2.559803 -2.913608 -2.814726 -3.267163 -3.110647	0.615515 -0.603745 -0.568320 0.613598 2.736411 2.721906 -1.531673 0.623007 1.652692 0.273982 -0.229649 0.040310	-0.272815 -0.362780 -0.184139 0.076683 0.364845 0.060080 -0.558592 -0.457975 -0.379350 -1.460886 0.554218 1.593017
С С Н Н С Н С Н С	-1.057851 -0.360557 1.000899 1.682905 1.559438 -0.914503 -0.877855 -2.559803 -2.913608 -2.814726 -3.267163 -3.110647 -4.033144	0.615515 -0.603745 -0.568320 0.613598 2.736411 2.721906 -1.531673 0.623007 1.652692 0.273982 -0.229649 0.040310 -1.276571	-0.272815 -0.362780 -0.184139 0.076683 0.364845 0.060080 -0.558592 -0.457975 -0.379350 -1.460886 0.554218 1.593017 0.259066
С С Н Н С Н С Н С Н	-1.057851 -0.360557 1.000899 1.682905 1.559438 -0.914503 -0.877855 -2.559803 -2.913608 -2.814726 -3.267163 -3.110647 -4.033144 -4.513636	0.615515 -0.603745 -0.568320 0.613598 2.736411 2.721906 -1.531673 0.623007 1.652692 0.273982 -0.229649 0.040310 -1.276571 -1.860933	-0.272815 -0.362780 -0.184139 0.076683 0.364845 0.060080 -0.558592 -0.457975 -0.379350 -1.460886 0.554218 1.593017 0.259066 1.030061
С С Н Н С Н С Н С Н Н	-1.057851 -0.360557 1.000899 1.682905 1.559438 -0.914503 -0.877855 -2.559803 -2.913608 -2.814726 -3.267163 -3.110647 -4.033144 -4.513636 -4.204013	0.615515 -0.603745 -0.568320 0.613598 2.736411 2.721906 -1.531673 0.623007 1.652692 0.273982 -0.229649 0.040310 -1.276571 -1.860933 -1.576855	-0.272815 -0.362780 -0.184139 0.076683 0.364845 0.060080 -0.558592 -0.457975 -0.379350 -1.460886 0.554218 1.593017 0.259066 1.030061 -0.766547
С С Н Н С Н С Н С Н С Н С Н С Н С Н	-1.057851 -0.360557 1.000899 1.682905 1.559438 -0.914503 -0.877855 -2.559803 -2.913608 -2.814726 -3.267163 -3.110647 -4.033144 -4.513636 -4.204013 1.899162	0.615515 -0.603745 -0.568320 0.613598 2.736411 2.721906 -1.531673 0.623007 1.652692 0.273982 -0.229649 0.040310 -1.276571 -1.860933 -1.576855 -1.605539	-0.272815 -0.362780 -0.184139 0.076683 0.364845 0.060080 -0.558592 -0.457975 -0.379350 -1.460886 0.554218 1.593017 0.259066 1.030061 -0.766547 -0.269373
С С Н Н С Н С Н С Н С Н Н С Н Н С О О	-1.057851 -0.360557 1.000899 1.682905 1.559438 -0.914503 -0.877855 -2.559803 -2.913608 -2.814726 -3.267163 -3.110647 -4.033144 -4.513636 -4.204013 1.899162 3.031385	0.615515 -0.603745 -0.568320 0.613598 2.736411 2.721906 -1.531673 0.623007 1.652692 0.273982 -0.229649 0.040310 -1.276571 -1.860933 -1.576855 -1.605539 0.357382	-0.272815 -0.362780 -0.184139 0.076683 0.364845 0.060080 -0.558592 -0.457975 -0.379350 -1.460886 0.554218 1.593017 0.259066 1.030061 -0.766547 -0.269373 0.162262
С С Н Н С Н С Н С Н С Н С Н Н О О С	-1.057851 -0.360557 1.000899 1.682905 1.559438 -0.914503 -0.877855 -2.559803 -2.913608 -2.814726 -3.267163 -3.110647 -4.033144 -4.513636 -4.204013 1.899162 3.031385 3.123575	0.615515 -0.603745 -0.568320 0.613598 2.736411 2.721906 -1.531673 0.623007 1.652692 0.273982 -0.229649 0.040310 -1.276571 -1.860933 -1.576855 -1.605539 0.357382 -1.067869	-0.272815 -0.362780 -0.184139 0.076683 0.364845 0.060080 -0.558592 -0.457975 -0.379350 -1.460886 0.554218 1.593017 0.259066 1.030061 -0.766547 -0.269373 0.162262 0.239318
С С Н Н С Н С Н С Н Н О О С Н	-1.057851 -0.360557 1.000899 1.682905 1.559438 -0.914503 -0.877855 -2.559803 -2.913608 -2.814726 -3.267163 -3.110647 -4.033144 -4.513636 -4.204013 1.899162 3.031385 3.123575 3.239900	0.615515 -0.603745 -0.568320 0.613598 2.736411 2.721906 -1.531673 0.623007 1.652692 0.273982 -0.229649 0.040310 -1.276571 -1.860933 -1.576855 -1.605539 0.357382 -1.067869 -1.365593	-0.272815 -0.362780 -0.184139 0.076683 0.364845 0.060080 -0.558592 -0.457975 -0.379350 -1.460886 0.554218 1.593017 0.259066 1.030061 -0.766547 -0.269373 0.162262 0.239318 1.285256

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

		SF2a	
	Х	Y	Z
С	0.465897	1.626294	-0.126641
С	-0.812949	1.069101	-0.253902
С	-1.024327	-0.309929	-0.250098
С	0.066030	-1.184028	-0.107084
С	1.318397	-0.625181	0.011358
С	1.516673	0.746959	0.001221
Н	0.621381	2.694447	-0.122926
Н	-1.663728	1.727981	-0.354648
Н	-0.070895	-2.255575	-0.089826
С	-2.423451	-0.867388	-0.416349
Н	-2.772498	-0.701815	-1.437956
Н	-2.385242	-1.948655	-0.268872
С	-3.407654	-0.268931	0.543857
Н	-3.179609	-0.395275	1.596645
С	-4.500419	0.401116	0.187809
Н	-5.175158	0.814066	0.923349
Н	-4.752483	0.552548	-0.853690
0	2.521206	-1.262044	0.207859
0	2.851455	1.020906	0.193112
С	3.504145	-0.239219	0.016985
Н	3.895395	-0.303375	-1.002463
Н	4.287501	-0.348013	0.759679
		SF2b	
	Х	Y	Z
С	0.481934	1.637630	-0.172898
С	-0.802811	1.096983	-0.308455
С	-1.029514	-0.279535	-0.329586
С	0.050773	-1.168255	-0.204371
С	1.308044	-0.625342	-0.062582
С	1.521415	0.744224	-0.047619
Н	0.651328	2.703642	-0.166887
Н	-1.647152	1.766964	-0.390256
Н	-0.096228	-2.238415	-0.222928
С	-2.438467	-0.813725	-0.484910
Н	-2.839844	-0.531074	-1.460177
Н	-2.401700	-1.904696	-0.462443
С	-3.363202	-0.323431	0.589772
Н	-3.076558	-0.564194	1.607735
С	-4.469130	0.383209	0.371881
Н	-5.097139	0.715581	1.185468
Н	-4.779233	0.647003	-0.630830
0	2.513806	-1.279785	0.030792
0	2.869822	0.999476	0.053261
С	3.447565	-0.260909	0.403534
Н	4.372611	-0.400269	-0.146008
Н	3.605258	-0.297169	1.485323

		SF3a	
	Х	Y	Z
С	0.616119	1.764116	0.177236
С	-0.711869	1.523465	-0.204429
С	-1.157148	0.259572	-0.585554
С	-0.262043	-0.825175	-0.591761
С	1.038711	-0.576987	-0.222302
С	1.470655	0.687325	0.154121
Н	0.952768	2.745566	0.474460
Н	-1.412734	2.346730	-0.202949
Н	-0.585415	-1.817575	-0.870764
С	-2.599348	0.035085	-0.951610
Н	-3.024793	0.959598	-1.349956
Н	-2.665466	-0.691851	-1.765646
С	-3.472687	-0.441093	0.181143
Н	-4.506604	-0.631076	-0.087127
С	-3.087596	-0.635150	1.439076
Н	-3.788289	-0.976499	2.186827
Н	-2.069539	-0.459206	1.755833
0	2.079625	-1.468729	-0.112848
0	2.797257	0.632283	0.513986
С	3.240274	-0.649950	0.060972
Н	3.747649	-0.536759	-0.901328
Н	3.886960	-1.094600	0.810193
		SF3b	
	Х	Y	Ζ
С	0.615494	1.765506	0.213812
С	-0.719858	1.534059	-0.146805
С	-1.165481	0.288161	-0.583234
С	-0.262920	-0.786736	-0.670501
С	1.042140	-0.550794	-0.308323
С	1.474124	0.695318	0.124873
Н	0.955824	2.736567	0.539614
Н	-1.427556	2.348674	-0.079326
Н	-0.583153	-1.761834	-1.008062
С	-2.616040	0.069349	-0.917711
Н	-3.058238	1.007375	-1.262691
Н	-2.700445	-0.621767	-1.760804
С	-3.453911	-0.462427	0.216960
Н	-4.494234	-0.646872	-0.029510
С	-3.031230	-0.709945	1.453281
Н	-3.707843	-1.088755	2.205163
Н	-2.005165	-0.541576	1.747592
0	2.110484	-1.415229	-0.355765
0	2.828668	0.655776	0.361616
С	3.154290	-0.736755	0.349661
Н	4.095777	-0.883652	-0.169094
	2 102151	-1 106950	1 378229

		SF1a	SF1b	SF2a	SF2b	SF3a	SF3b
				Bo	nds		
	MUE	0.005	0.005	0.005	0.005	0.005	0.005
B3LYP	MAX	0.007	0.007	0.007	0.007	0.008	0.008
	MUE	0.004	0.004	0.004	0.004	0.004	0.004
B3LYP-D3	MAX	0.006	0.006	0.006	0.006	0.006	0.006
DODL VD <sup>d</sup>	MUE	0.001	0.001	0.001	0.001	0.001	0.001
B2PLYP	MAX	0.003	0.003	0.003	0.003	0.004	0.004
				An	gles		
	MUE	0.3	0.2	0.2	0.2	0.3	0.3
B3LYP	MAX	1	1	0.9	1	1.2	1.2
	MUE	0.1	0.1	0.1	0.1	0.1	0.1
BSLIP-DS	MAX	0.6	0.6	0.6	0.6	0.6	0.6
	MUE	0.1	0.1	0.1	0.1	0.1	0.1
B2PLYP	MAX	0.4	0.4	0.2	0.3	0.4	0.5
				Dista	ances		
D2LVD	MUE	0.035	0.036	0.037	0.038	0.044	0.045
BOLIP	MAX	0.090	0.088	0.091	0.091	0.105	0.107
D2LVD D2	MUE	0.015	0.015	0.015	0.021	0.014	0.014
DOLIF-DO	MAX	0.029	0.032	0.030	0.060	0.025	0.027
DODI VD	MUE	0.014	0.014	0.013	0.013	0.016	0.017
D2PLIP	MAX	0.038	0.038	0.036	0.036	0.040	0.040
				Rotational	l Constants		
	Ae	0.7	0.9	0.1	0.6	0.1	0.3
B3LYP	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
	Ae	0.5	0.3	0.3	1.9	0.6	0.3
B3LYP-D3	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
	Ae	1.2	1.4	0.1	1	0.6	0.8
B2PLYP	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

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

<sup>*a*</sup> Mean Unsigned Error (MUE), Maximum Absolute Error (MAX) with respect to the B2PLYP-D3

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

<sup>c</sup> Computed with SNSD basis set.

<sup>*d*</sup> Computed with 6-311++G(2d,2p) basis set

Table S4.	Harmonic vibrational	frequencies and I	R intensities	of safrol	conformers,	computed	at different	level of	theory:	B2PLYP-D3,
B2PLYP,	B3LYP-D3 and B3LY	Р.								

		D DI VD	SF1a	DODI VD/6 2	11 + C(2d 2n)	D2I VD I	2/SNSD	D2I VD	SNCD
Mode	Approximate Description	V	I I	V	II++0(20,2p) I	v	I	v	I
1	$\tau CC(R)CH_2+\gamma C(R)-C+\delta CH_2$	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	$\tau CCCC(R) + \tau COCC(OX) + \tau CCC = C$	211	0	209	0	210	0	210	0
6	$\tau COCC(OX) + \delta CCC + \tau CCCC(R)$	255	1	254	1	250	1	250	1
7	$\delta$ CCC+ $\delta$ CC=C+ $\tau$ COCC(OX)	288	2	288	2	287	2	285	2
8	$\tau COCC(OX) + \delta CCC(R) + \tau CCCC(R)$	363	0	360	0	358	0	358	0
9	$\delta CC=C+\tau CCCC(R)$	393	1	390	1	390	1	385	1
10	$\tau CCCC(R) + \delta CCC(R)$	430	6	429	6	429	6	429	6
11	$\delta CCC(R) + \tau CCCC(R) + \delta CCC$	455	3	453	3	453	3	451	3
12	$\delta CCC(R) + \delta CC = C + \delta CH(R)$	498	1	497	2	496	1	496	2
13	t=CH <sub>2</sub> +γCH	603	7	600	7	601	8	599	7
14	$\tau CCCC(R) + \delta CCC(R) + t = CH_2 + \gamma CH$	619	7	615	7	617	7	617	7
15	$t=CH_2+\gamma CH+\delta CCC(R)+\tau CCCC(R)$	678	10	675	10	676	9	673	9
16	δCOC+δCCC(R)	729	3	727	3	732	3	729	4
17		742	0	/38	1	740	I 16	740	I
18		792	1/	/88	18	/88	16	/8/	16
19		824	24	817	25	823	20	821	25
20		833	10	020 876	13	052 002	15	851	17
21		007	8	016	14 8	003	0	002	12
22	8000 + 2012 + 201	030	2	020	1	037	24	908	20
23	$\alpha CH(P) + \alpha - CH_{2}$	939	2	929	37	937	15	933	13
24	$\gamma C \Gamma(R) + \omega - C H_2$	949	32 46	945	50	939	13	940	17
25		956	40	953	1	951	14	948	16
20	$vCH + r-CH_2 + vCC + vCO$	964	15	959	8	962	24	962	28
28	$\gamma CH + t = CH_2$	1038	21	1033	22	1026	20	1026	21
29	vCO+8CH	1067	115	1060	115	1064	114	1062	113
30	δCH(R)+δCH+vCC(R)+ vCO	1114	15	1112	14	1109	14	1107	15
31	s-CH <sub>2</sub> +δCH+vCC(R)	1130	6	1130	6	1123	6	1121	6
32	r-CH <sub>2</sub> (OX)+δCH(R)	1143	8	1142	7	1137	8	1136	9
33	$\delta CH(R)+r-CH_2(OX)$	1157	10	1154	9	1143	14	1143	12
34	$t-CH_2(OX)+\delta CH(R)+\delta CH+\nu CC(R)+\nu CO$	1207	23	1206	25	1199	18	1198	18
35	t-CH <sub>2</sub> (OX)+ vCC(R)+ vCO	1235	16	1234	17	1220	17	1219	14
36	$t-CH_2 + vCC(R) + vCO$	1240	2	1242	5	1230	2	1228	3
37	$vCC(R)+t-CH_2$	1283	252	1277	266	1279	253	1276	262
38	$t-CH_2+\delta CH(R)$	1296	28	1300	11	1287	30	1288	26
39	$t-CH_2+\nu CC(R)+\delta CCH(R)$	1324	3	1327	2	1316	3	1316	3
40	$\omega$ -CH <sub>2</sub> + $\delta$ CH+ $\delta$ CCH(R)	1335	2	1338	2	1328	2	1328	2
41	$\delta CH + t - CH_2$	1411	5	1403	10	1404	11	1399	12
42	ω–CH <sub>2</sub> (OX)	1435	2	1435	2	1425	2	1425	2
43	$s=CH_2+\delta CH+s-CH_2$	1462	2	1466	6	1447	2	1447	2
44	s=CH <sub>2</sub> +vCC(R)+δCCC(R)+t-CH <sub>2</sub> + $ω$ - CH <sub>2</sub> (OX)	1477	59	1472	59	1469	18	1466	22
45	s-CH <sub>2</sub>	1492	33	1495	27	1477	75	1475	66
46	$\delta CCH(R) + \nu CC(R) + s-CH_2(OX)$	1525	192	1524	180	1523	180	1522	191
47	s-CH <sub>2</sub> (OX)	1555	6	1554	4	1538	33	1538	26
48	$vCC(R) + \delta CCC(R)$	1653	5	1645	5	1653	5	1649	5
49	$vCC(R) + \delta CCC(R)$	1669	1	1662	1	1672	2	1669	1
50	vC=C+s=CH	1699	13	1693	13	1704	15	1700	15
51	v C <sub>20</sub> H <sub>21</sub>	3026	116	3039	113	3003	128	3000	129
52	V <sub>s</sub> СП <sub>2</sub>	2081	23	304/ 2096	23	3013	24	2040	12
55		2150	11	3080	11	2119	12	3112	12
54		3150	13	3152	12	2127	32	3115	35 14
33 56		3150	∠0 1	3166	5 25	3127	15	3123	14 1
50		3109	4 Q	3105	23	3130	9	3154	4
58		3792	2	3215	1	3198	2	3194	2
59	VCH(R)	3223	4	3226	4	3206	4	3204	4
60	v=CH-	3240	14	3244	13	3217	15	3215	15
00	v <sub>as</sub> =OT <sub>2</sub>	5240	14	J244	15	3417	13	5415	15

		B2PLYP-	D3/Maug	B2PLYP/6-31	1++G(2d,2p)	B3LYP-I	D3/SNSD	B3LYP	/SN
Mode	Approximate Description	v	I	v	I	v	Ι	v	
1	$\tau CC(R)CH_2+\gamma C(R)-C+\delta CH_2$	30	0	30	0	30	0	28	
2	τCCC=C	72	0	72	0	71	0	71	
3	TCOCC(OX)	107	3	107	3	100	5	100	
4		150	8	149	8	133	4	131	
5	TCCCC(R)+TCOCC(OX)+TCCC=C	212	0	211	0	212	0	212	
6		253	1	252	1	248	1	249	
7		285	1	285	1	284	1	283	
8	TCOCC(0X)+8CCC(R)+TCCCC(R)	369	1	367	1	363	1	362	
9	8CC-C+ 7CCCC(R)	391	1	389	1	389	1	385	
10		431	6	431	6	430	6	431	
11	8CCC(R)++CCCC(R)+8CCC	449	3	448	3	449	3	447	
12	8CCC(R)+8CC-C+8CH(R)	498	2	497	2	496	1	495	
12		606	7	603	8	603	9	601	
14		616	7	612	6	614	5	614	
14		691	0	678	0	679	0	675	
16	SCOC (SCCC(R))	720	2	728	2	722	2	720	
10		750	5	726	3	732	5	730	
10		741	17	730	1	739	17	759	
18		192	17	789	18	/00	17	/8/	
19		825	28	819	31	824	30	823	
20	τCCCC(R) +γCH	833	16	826	12	831	13	829	
21	γCH	887	14	876	15	882	13	882	
22	$r=CH_2+r-CH_2+\gamma CH$	916	5	916	5	909	7	907	
23	$\delta CCC + \gamma CH + \omega = CH_2$	939	2	928	3	937	30	935	
24	$\gamma CH(R) + \omega = CH_2$	949	33	943	37	939	8	940	
25	$\nu$ CO+ $\gamma$ CH+ $\omega$ =CH <sub>2</sub>	954	48	947	50	947	20	945	
26	$\omega = CH_2$	956	2	953	1	951	15	948	
27	$\gamma$ CH + r-CH <sub>2</sub> + $\nu$ CC+ $\nu$ CO	965	14	959	8	963	23	963	
28	$\gamma CH + t = CH_2$	1037	20	1033	21	1026	20	1026	
29	νCO+δCH	1067	113	1059	113	1064	112	1062	
30	$\delta CH(R) + \delta CH + vCC(R) + vCO$	1114	15	1112	15	1108	15	1106	
31	$s-CH_2+\delta CH+\nu CC(R)$	1129	6	1129	6	1122	6	1120	
32	$r-CH_2(OX)+\delta CH(R)$	1144	8	1142	7	1137	8	1136	
33	$\delta CH(R)+r-CH_2(OX)$	1157	11	1154	10	1143	14	1143	
34	$t-CH_2(OX)+\delta CH(R)+\delta CH+\nu CC(R)+\nu CO$	1207	24	1206	25	1199	18	1198	
35	$t-CH_2(OX)+\nu CC(R)+\nu CO$	1235	17	1233	18	1220	17	1219	
36	$t-CH_2 + \nu CC(R) + \nu CO$	1239	2	1241	6	1229	3	1227	
37	$vCC(R)+t-CH_2$	1283	252	1277	265	1279	251	1276	
38	$t-CH_2+\delta CH(R)$	1297	28	1301	11	1288	31	1288	
39	ω-CH <sub>2</sub> +δCH+δCCH(R)	1324	3	1327	2	1316	3	1316	
40	$\delta CH + t - CH_2$	1335	2	1338	2	1328	1	1328	
41	$t-CH_2+\nu CC(R)+\delta CCH(R)$	1411	5	1403	10	1404	11	1399	
42	ω–CH <sub>2</sub> (OX)	1435	2	1435	2	1425	2	1425	
43	$s=CH_2+\delta CH+s-CH_2$	1462	2	1466	5	1447	2	1447	
44	$\begin{array}{c} s{=}CH_2{+}\nuCC(R){+}\deltaCCC(R){+}t{-}CH_2{+}\;\omega{-}\\ CH_2(OX) \end{array}$	1477	61	1472	62	1469	19	1466	
45	s-CH <sub>2</sub>	1492	31	1495	26	1477	73	1475	
46	$\delta CCH(R) + vCC(R) + s-CH_2(OX)$	1525	192	1524	181	1523	181	1522	
47	s-CH <sub>2</sub> (OX)	1555	6	1553	4	1538	32	1539	
48	$vCC(R) + \delta CCC(R)$	1653	5	1645	5	1653	5	1649	
49	$\nu$ CC(R) + $\delta$ CCC(R)	1669	1	1662	1	1672	2	1669	
50	vC=C + s=CH	1698	13	1692	13	1704	16	1700	
51	$v C_{20}H_{21}$	3026	114	3039	112	3003	127	3001	
52	$v_s CH_2$	3041	22	3047	21	3013	23	3010	
53	$v_{as} CH_2$	3082	11	3087	11	3054	12	3049	
54	$v_{as} CH_2(OX)$	3150	13	3152	13	3118	33	3113	
55	vCH	3152	29	3162	5	3127	14	3125	
56	$v_s = CH_2 + vCH$	3159	4	3165	26	3136	5	3134	
57	vCH(R)	3192	9	3195	8	3175	9	3172	
58	vCH(R)	3212	1	3215	1	3197	2	3194	
59	vCH(R)	3223	4	3226	4	3206	4	3204	
60	v =CH-	3240	13	3244	13	3217	15	3215	

M. 1		B2PLYP-	D3/Maug	B2PLYP/6-31	1++G(2d,2p)	B3LYP-I	D3/SNSD	B3LYP	/SNS
Mode	Approximate Description	v	I	v	I	v	Ι	v	
1	$\tau CC(R)CH_2+\gamma C(R)-C+\delta CH_2$	20	0	19	0	22	0	19	
2	τCCC=C	79	0	79	0	79	0	78	
3	τCOCC(OX)	110	3	110	3	105	6	104	
4	τCOCC(OX)	150	7	151	8	135	4	133	
5	TCCCC(R)+TCOCC(OX)+TCCC=C	218	0	216	0	216	0	216	
6	τCOCC(OX)+δCCC+τCCCC(R)	246	1	247	1	242	1	244	
7	$\delta CCC + \delta CC = C + \tau COCC(OX)$	279	3	277	3	276	2	274	
8	τCOCC(OX)+δCCC(R)+τCCCC(R)	356	0	354	0	352	0	351	
9	$\delta CC = C + \tau CCCC(R)$	390	1	388	1	387	1	384	
10		434	5	434	5	433	5	434	
11		446	5	445	5	445	5	443	
12	δCCC(R)+δCC=C+δCH(R)	509	4	508	4	508	4	507	
13	t=CHo+vCH	606	9	602	9	603	10	601	
14		612	6	609	6	611	5	610	
15		684	0	681	9	681	8	678	
15	SCOC ( SCCC (R)	728	1	727	2	731	2	720	
17		720	1	727	1	731	1	741	
10		744	1	740	1	796	1	741	
10		790	0	/8/	/	/80	20	/ 64	
19	VCC(R) + VCO	827	16	821	19	827	20	824	
20	γCH+τCCCCC(R)	835	24	828	19	831	18	831	
21	γCH	878	13	869	14	874	12	875	
22	$r=CH_2+r-CH_2+\gamma CH$	922	11	922	10	915	14	913	
23	$ω = CH_2 + ω - CH_2 + γCH$	928	15	926	16	922	13	919	
24	$vCO+\gamma CH+\omega=CH_2$	951	8	940	2	939	37	940	
25	$\gamma CH + \omega = CH_2$	953	31	945	37	950	1	949	
26	$\omega = CH_2$	956	53	949	50	955	49	954	
27	vCC + vCO	975	8	971	8	971	9	968	
28	$\gamma CH + t = CH_2$	1037	19	1032	20	1025	20	1026	
29	νCO+δCH	1067	128	1060	129	1064	126	1062	
30	$\delta CH(R) + \delta CH + \nu CC(R) + \nu CO$	1116	16	1113	15	1112	15	1109	
31	s-CH <sub>2</sub> + $\delta$ CH+ $\nu$ CC(R)	1129	1	1130	1	1121	1	1119	
32	$r-CH_2(OX)+\delta CH(R)$	1150	6	1149	5	1140	7	1140	
33	$\delta CH(R)+r-CH_2(OX)$	1158	12	1155	11	1148	15	1146	
34	$t-CH_2(OX)+\delta CH(R)+\delta CH+\nu CC(R)+\nu CO$	1204	26	1204	27	1196	20	1195	
35	$t-CH_2(OX)+\nu CC(R)+\nu CO$	1235	11	1234	13	1220	11	1219	
36	$t-CH_2 + \nu CC(R) + \nu CO$	1243	22	1244	29	1234	23	1231	
37	$vCC(R)+t-CH_2$	1287	245	1281	250	1280	230	1279	
38	$t-CH_2+\delta CH(R)$	1302	9	1305	5	1296	20	1295	
39	ω-CH <sub>2</sub> +δCH+δCCH(R)	1320	29	1325	19	1312	38	1312	
40	$\delta CH + t - CH_2$	1333	6	1336	7	1327	8	1327	
41	$t-CH_2+vCC(R)+\delta CCH(R)$	1403	3	1395	6	1396	7	1392	
42	ω–CH <sub>2</sub> (OX)	1434	2	1434	2	1424	2	1424	
43	$s=CH_2+\delta CH+s-CH_2$	1462	1	1467	1	1448	1	1448	
44	$\begin{array}{c} s{=}CH_2{+}\nuCC(R){+}\deltaCCC(R){+}t{-}CH_2{+}\;\omega{-}\\ CH_2(OX) \end{array}$	1479	58	1474	55	1472	27	1470	
45	s-CH <sub>2</sub>	1492	7	1495	8	1476	41	1474	
46	$\delta CCH(R) + vCC(R) + s-CH_2(OX)$	1527	206	1526	197	1524	180	1523	
47	s-CH <sub>2</sub> (OX)	1554	8	1553	6	1538	49	1538	
48	$\nu$ CC(R) + $\delta$ CCC(R)	1650	9	1643	9	1651	9	1647	
49	$\nu$ CC(R) + $\delta$ CCC(R)	1668	0	1662	1	1671	0	1668	
50	$vC=C+s=CH_2$	1699	14	1693	14	1704	17	1700	
51	$v C_{20}H_{21}$	3025	119	3038	115	3002	131	2999	
52	$v_s CH_2$	3039	23	3046	23	3011	25	3008	
53	$v_{as} CH_2$	3077	11	3083	10	3048	12	3045	
54	$v_{as} CH_2(OX)$	3150	13	3152	12	3119	33	3114	
55	vCH	3153	28	3162	5	3127	13	3126	
56	$v_s = CH_2 + vCH$	3159	4	3166	26	3137	5	3134	
57	vCH(R)	3198	3	3201	3	3183	3	3180	
58	vCH(R)	3208	4	3212	4	3191	4	3188	
59	vCH(R)	3223	3	3226	3	3206	4	3203	
(0)		22.41	14	2210	12	2230		2205	

		B2PLYP-	D3/Maug	B2PLYP/6-31	1++G(2d,2p)	B3LYP-I	D3/SNSD	B3LYP	SNS
Mode	Approximate Description	v	I	v	I	v	Ι	v	
1	$\tau CC(R)CH_2+\gamma C(R)-C+\delta CH_2$	15	0	19	0	20	0	14	
2	τCCC=C	78	0	78	0	78	0	77	
3	τCOCC(OX)	110	3	107	3	103	6	103	
4	τCOCC(OX)	150	8	150	9	134	4	132	
5	TCCCC(R)+TCOCC(OX)+TCCC=C	216	0	213	0	213	0	214	
6		253	1	253	1	245	0	248	
7	80000(0X)100000100000(X)	271	0	269	0	273	0	268	
8	TCOCC(0X)+8CCC(B)+TCCCC(B)	365	2	363	2	358	1	359	
9		385	1	383	- 1	384	1	380	
10		134	5	432	5	432	5	/33	
11	\$CCC(R)+0CCC(R)	447	5	432	5	432	5	433	
12		447 507	2	440 506	3	440 507	2	506	
12		507	5	506	4	507	3	506	
13	$t=CH_2+\gamma CH$	606	5	604	6	605	13	602	
14	$\tau CCCC(R) + \delta CCC(R) + t = CH_2 + \gamma CH$	610	11	605	11	607	3	607	
15	$t=CH_2+\gamma CH+\delta CCC(R)+\tau CCCC(R)$	685	7	682	7	683	6	679	
16	$\delta COC + \delta CCC(R)$	729	1	728	1	732	1	729	
17	τCCCC(R)	742	1	738	1	740	1	740	
18	$vCC(R)$ + $vCO$ + $\delta CCC$	790	8	787	9	786	7	785	
19	νCC(R)+ νCO	827	17	822	24	828	24	825	
20	γCH+τCCCC(R)	834	21	827	14	830	14	830	
21	γCH	879	15	870	15	874	14	876	
22	$r=CH_2+r-CH_2+\gamma CH$	922	8	922	10	914	12	912	
23	$ω=CH_2+ω-CH_2+γCH$	929	13	927	11	922	12	920	
24	$vCO+\gamma CH+\omega=CH_2$	949	15	937	9	939	37	940	
25	$\gamma CH + \omega = CH_2$	952	25	944	32	949	3	948	
26	ω=CH <sub>2</sub>	956	54	949	50	955	46	955	
27	vCC + vCO	974	8	970	7	970	9	967	
28	$\gamma CH + t = CH_2$	1036	19	1031	20	1025	20	1025	
29	νCO+δCH	1067	126	1059	126	1064	125	1062	
30	$\delta CH(R) + \delta CH + vCC(R) + vCO$	1117	17	1114	16	1112	16	1110	
31	s-CH_+&CH+vCC(R)	1126	1	1127	1	1120	1	1117	
32	r-CH.(OX)+8CH(R)	1150	5	11/18	4	11/0	6	1140	
32	8CH(R)+r-CH (OX)	1150	13	1155	12	1140	16	1146	
24		1205	15	1204	12	1140	20	1140	
34 25		1205	28	1204	27	1210	20	1210	
35	$I = CH_2(OX) + VCC(R) + VCO$	1235	12	1234	13	1219	11	1219	
36	$t - CH_2 + vCC(R) + vCO$	1241	22	1241	28	1233	23	1229	
37	$vCC(R)+t-CH_2$	1288	246	1281	250	1281	230	1279	
38	$t-CH_2+\delta CH(R)$	1303	5	1306	4	1296	18	1296	
39	ω-CH <sub>2</sub> +δCH+δCCH(R)	1320	29	1324	18	1313	39	1312	
40	$\delta CH + t - CH_2$	1333	7	1336	8	1327	8	1327	
41	$t-CH_2+\nu CC(R)+\delta CCH(R)$	1403	3	1395	6	1396	7	1391	
42	ω–CH <sub>2</sub> (OX)	1434	2	1434	2	1424	2	1424	
43	$s=CH_2+\delta CH+s-CH_2$	1462	1	1467	1	1448	1	1448	
44	s=CH <sub>2</sub> +vCC(R)+δCCC(R)+t-CH <sub>2</sub> + $ω$ - CH <sub>2</sub> (OX)	1479	58	1474	56	1472	27	1469	
45	s-CH <sub>2</sub>	1493	6	1496	7	1477	40	1474	
46	$\delta$ CCH(R)+ $\nu$ CC(R)+ s-CH <sub>2</sub> (OX)	1528	205	1526	199	1525	182	1524	
47	s-CH <sub>2</sub> (OX)	1554	8	1553	6	1538	47	1539	
48	$vCC(R) + \delta CCC(R)$	1650	9	1642	9	1650	9	1646	
49	$vCC(R) + \delta CCC(R)$	1669	0	1662	1	1671	0	1668	
50	$vC=C+s=CH_2$	1698	14	1692	14	1704	17	1700	
51	v C <sub>20</sub> H <sub>21</sub>	3025	117	3038	114	3002	130	2999	
52	v. CH2	3042	23	3048	22	3012	23	3010	
53	v CH <sub>2</sub>	3081	10	3086	10	3050	12	3048	
54	$v_{as} O v_{2}$	3150	13	3152	13	3110	3/	3114	
55		3152	20	3162	5	3117	14	3174	
		2150	29	2167	3	3127	14	3120	
56	$v_s = UH_2 + vUH$	3159	4	316/	26	5136	5	5154	
57	vCH(R)	3197	4	3199	5	3183	3	3178	
58	vCH(R)	3208	4	3212	4	3192	4	3189	
59	vCH(R)	3223	3	3226	3	3206	4	3203	
60	$v_{\rm ex} = CH_{\rm e}$	3241	14	3244	13	3217	15	3215	

Mode	Approvimate Description	B2PLYP-	D3/Maug	B2PLYP/6-31	11++G(2d,2p)	B3LYP-I	03/SNSD	B3LYP	/SI
Mode	Approximate Description	v	Ι	v	Ι	v	Ι	v	
1	$\tau CC(R)CH_2 + \gamma C(R) - C + \delta CH_2$	38	0	37	0	36	0	36	
2	τCCC=C	77	1	78	1	75	2	77	
3	τCOCC(OX)	130	0	132	0	117	7	116	
4	τCOCC(OX)	138	9	138	9	130	0	128	
5		198	1	197	1	195	1	193	
6	rcocc(0X)+80000(0X)+80000-0	255	1	253	1	249	0	247	
7		203	1	290	1	242	1	247	
8	*COCC(0X)+&CCC(B)+*CCCC(B)	354	1	352	1	349	0	346	
9	8CC-C+ + + CCCC(P)	/13	1	412	1	412	1	/09	
10		430	4	412	1	412	4	129	
11	\$CCC(P) + -CCCC(P) + \$CCC	456	-	453		455		452	
12		560	4	558	1	558	4	557	
12		560	4	568	12	562	12	563	
15		509	14	508	15	305 615	15	505	
14	$t \cup U \cup U \mid s \cap U \mid s \cap C \cap$	615	3	612	4	615	3	612	
15	$ω = CH_2 + γCH + δCCC(R) + τCCCC(R)$	673	10	6/1	9	6/1	9	670	
16	SCOC+SCCC(R)	728	2	726	2	730	2	728	
17		745	1	739	1	740	2	/40	
18	$vCC(R) + vCO + \delta CCC$	778	9	775	10	776	9	774	
19	vCC(R)+ vCO	825	19	820	20	826	21	823	
20	τCCCC(R) +γCH	836	19	828	17	832	15	831	
21	γCH	883	12	873	13	878	12	878	
22	νCC+ νCO+ γCH	915	11	910	10	910	11	907	
23	$vCC+ vCO+ r-CH_2$	942	8	931	1	934	15	932	
24	γCH(R)	944	2	940	10	941	0	942	
25	$\nu$ CO+ $\gamma$ CH+ $\omega$ =CH <sub>2</sub>	954	15	947	22	946	5	945	
26	$ω=CH_2$	959	59	951	51	954	57	954	
27	$\gamma CH + r - CH_2$	976	3	973	2	969	7	968	
28	$\gamma CH + t = CH_2$	1040	14	1037	15	1027	14	1029	
29	νCO+δCH	1067	119	1059	119	1064	117	1062	
30	$r=CH_2+\delta CH$	1078	2	1080	2	1071	1	1070	
31	$\delta CH(R) + \delta CH + \nu CC(R) + \nu CO$	1122	16	1120	15	1117	16	1115	
32	$r-CH_2(OX)+\delta CH(R)$	1146	7	1145	6	1139	8	1138	
33	$\delta CH(R)+r-CH_2(OX)$	1158	9	1154	8	1145	10	1144	
34	$t-CH_2(OX)+\delta CH(R)+\delta CH+\nu CC(R)+\nu CO$	1207	5	1208	13	1197	3	1197	
35	$t-CH_2 + \nu CC(R) + \nu CO$	1215	33	1217	32	1205	26	1205	
36	t-CH <sub>2</sub> (OX)+ vCC(R)+ vCO	1236	20	1234	21	1221	25	1220	
37	$vCC(R)+t-CH_2$	1287	250	1280	248	1281	251	1279	
38	$t-CH_2+\delta CH(R)$	1305	10	1307	6	1298	12	1298	
39	δCH +t-CH <sub>2</sub>	1329	3	1334	3	1322	3	1322	
40	ω–CH <sub>2</sub> +δCH+δCCH(R)	1364	7	1367	4	1354	7	1355	
41	t-CH₂+vCC(R)+δCCH(R)	1410	7	1401	12	1403	13	1398	
42	ω-CH <sub>2</sub> (OX)	1435	2	1434	2	1425	2	1425	
43	s=CH <sub>2</sub> +δCH+s-CH <sub>2</sub>	1456	2	1461	2	1442	3	1442	
44	s-CH <sub>2</sub>	1480	83	1475	79	1472	19	- 1471	
45	s=CH <sub>2</sub> +νCC(R)+δCCC(R)+t-CH <sub>2</sub> + ω– CH <sub>2</sub> (OX)	1492	10	1495	11	1476	79	1473	
46	$\delta$ CCH(R)+ vCC(R)+ s-CH <sub>2</sub> (OX)	1528	173	1527	165	1526	148	1524	
47	s-CH <sub>2</sub> (OX)	1555	6	1553	5	1538	42	1539	
48	$vCC(R) + \delta CCC(R)$	1652	6	1645	6	1653	6	1648	
49	$vCC(R) + \delta CCC(R)$	1670	0	1663	0	1673	0	1670	
50	vC=C + s=CH <sub>2</sub>	1699	17	1694	17	1703	19	1702	
51	v C <sub>20</sub> H <sub>21</sub>	3026	118	3038	110	3003	130	3000	
52	v <sub>s</sub> CH <sub>2</sub>	3033	27	3039	31	3005	29	3002	
53	v CH2	3062	11	3067	10	3034	12	3029	
54	v <sub>ac</sub> CH <sub>2</sub> (OX)	3147	26	3150	26	3118	32	3113	
55	.as с. 12(СЛ)	3152	27	3166	25	3126	28	3122	
56	$v = CH_{*} + vCH$	3166	8	3168	8	3145	8	3143	
57	······································	3103	7	3106	7	3176	8	3173	
58		3700	2	3713	2	3104	3	3101	
50		2009	2	2006	2	2204	5	3204	
1.4		1//1		3 / / 1		3 (110)	<i>/</i> <b>/</b>		

			SF3b						
Mode	Approximate Description	B2PLYP-	D3/Maug	B2PLYP/6-3	11++G(2d,2p)	B3LYP-I	03/SNSD	B3LYP	/SNSD
		v	Ι	v	Ι	v	Ι	v	Ι
1	$\tau CC(R)CH_2 + \gamma C(R) - C + \delta CH_2$	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	$\tau COCC(OX) + \delta CCC + \tau CCCC(R)$	255	1	252	1	249	1	247	1
7	$\delta CCC + \delta CC = C + \tau COCC(OX)$	293	1	290	1	292	1	289	1
8	$\tau COCC(OX) + \delta CCC(R) + \tau CCCC(R)$	356	0	353	0	350	0	347	0
9	$\delta CC = C + \tau CCCC(R)$	415	2	414	2	414	2	411	2
10	$\tau CCCC(R) + \delta CCC(R)$	431	4	430	4	430	4	430	4
11	δCCC(R)+τCCCC(R)+δCCC	454	2	451	2	453	2	450	2
12	SCCC(R)+SCC=C+SCH(R)	559	5	557	5	557	5	556	5
13	$t=CH_2+\gamma CH$	570	13	568	13	564	13	563	12
14	$\tau CCCC(R) + \delta CCC(R) + t = CH_2 + \gamma CH$	611	2	608	2	611	2	609	2
15	$ω = CH_2 + \gamma CH + \delta CCC(R) + \tau CCCC(R)$	676	8	674	8	674	8	673	8
16	$\delta COC + \delta CCC(R)$	729	1	727	1	730	2	728	2
17	τCCCC(R)	742	2	737	1	740	2	739	2
18	vCC(R)+ vCO +δCCC	779	10	776	12	776	11	774	11
19	vCC(R)+ vCO	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	$vCC+ vCO+ r-CH_2$	941	13	931	4	934	18	932	16
24	γCH(R)	944	0	940	9	941	1	942	1
25	$\nu$ CO+ $\gamma$ CH+ $\omega$ =CH <sub>2</sub>	954	11	947	17	945	7	944	8
26	$\omega = CH_2$	958	62	950	56	954	54	954	51
27	$\gamma CH + r - CH_2$	976	3	973	3	969	7	968	11
28	$\gamma CH + t = CH_2$	1040	14	1037	15	1027	13	1029	14
29	νCO+δCH	1067	115	1059	115	1064	114	1062	114
30	$r=CH_{2}+\delta CH$	1078	2	1080	2	1071	2	1070	2
31	$\delta CH(R) + \delta CH + \nu CC(R) + \nu CO$	1122	15	1120	15	1117	15	1115	16
32	$r-CH_2(OX)+\delta CH(R)$	1147	3	1145	2	1139	3	1138	2
33	$\delta CH(R)+r-CH_2(OX)$	1158	12	1154	11	1146	14	1144	14
34	$t-CH_2(OX)+\delta CH(R)+\delta CH+\nu CC(R)+\nu CO$	1207	5	1208	13	1197	3	1197	4
35	$t-CH_2 + vCC(R) + vCO$	1215	33	1217	31	1205	26	1205	25
36	$t-CH_2(OX) + vCC(R) + vCO$	1236	20	1235	21	1222	24	1221	20
37	$vCC(R)+t-CH_2$	1286	249	1280	248	1281	250	1278	255
38	t–CH₂+δCH(R)	1305	10	1307	6	1298	11	1298	11
39	$\delta CH + t - CH_2$	1329	3	1334	3	1322	3	1322	2
40	ω-CH <sub>2</sub> +δCH+δCCH(R)	1364	7	1367	4	1354	7	1355	7
41	$t-CH_2+vCC(R)+\delta CCH(R)$	1410	7	1401	12	1403	13	1398	15
42	ω–CH <sub>2</sub> (OX)	1434	2	1434	2	1424	2	1424	2
43	$s=CH_2+\delta CH+s-CH_2$	1456	2	1461	2	1442	3	1442	2
44	s-CH <sub>2</sub>	1480	83	1475	78	1472	19	1471	34
45	$s=CH_2+vCC(R)+\delta CCC(R)+t-CH_2+\omega$	1491	10	1494	11	1476	79	1473	58
16	$CH_2(OX)$	1500	170	1507	1.7	1506	145	1504	164
46	$\delta CCH(R) + VCC(R) + S - CH_2(OX)$	1528	172	1527	167	1520	145	1524	164
47	S-CH <sub>2</sub> (OX)	1554	1	1553	5	1538	44	1538	33
48	$vCC(R) + \delta CCC(R)$	1652	6	1645	6	1653	6	1648	6
49	$vCC(R) + \delta CCC(R)$	1670	0	1663	0	1673	0	1670	0
50	$vC=C + s=CH_2$	1699	16	1694	17	1703	18	1702	19
51	v C <sub>20</sub> H <sub>21</sub>	3025	113	3038	127	3002	129	2999	133
52	v <sub>s</sub> CH <sub>2</sub>	3033	25	3039	7	3005	22	3001	18
53	v <sub>as</sub> CH <sub>2</sub>	3062	11	3067	10	3034	12	3029	11
54	v <sub>as</sub> CH <sub>2</sub> (OX)	3148	26	3150	26	3120	34	3114	34
55	vCH	3153	28	3166	27	3126	28	3122	29
56	$v_s = CH_2 + vCH$	3166	8	3167	7	3144	8	3143	7
57	vCH(R)	3193	7	3195	7	3176	8	3173	8
58	vCH(R)	3209	2	3212	2	3194	3	3190	3
59	vCH(R)	3223	3	3226	3	3206	4	3204	4
60	$v_{as}=CH_2$	3249	13	3252	13	3227	14	3225	14

<sup>a</sup> Abbreviations: v - bond stretching,  $\delta$  - bending, deformation in plane,  $\gamma$  - out-of-plane bending,  $\tau$  - torsion, s – scissoring, r – rocking,  $\omega$  - wagging, t – twisting, R– phenolic ring, OX-1,3-dioxolane ring.

<sup>b</sup> 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<sup>a</sup>, all values in cm<sup>-1</sup>.

		SF1a	SF1b	SF2a	SF2b	SF3a	SF3b
		I	Iarmonic				
D 21 VD <sup>b</sup>	MUE	10	10	10	10	10	10
BSLIP	MAX	36	37	36	36	35	33
	MUE	9	9	9	9	9	9
BSLIP-DS	MAX	31	32	31	31	30	28
	MUE	4	4	4	4	4	4
B2PLYP	MAX	13	13	13	13	13	13
B2PLYP-D3d	ZPVE	39032	39029	39026	39022	39036	39037
B3LYP	$\Delta ZPVE$	-297	-297	-298	-297	-301	-299
B3LYP-D3	$\Delta ZPVE$	-248	-248	-247	-246	-253	-250
B2PLYP	$\Delta ZPVE$	-39	-38	-36	-37	-36	-41
		Aı	nharmoni	c			
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	$\Delta ZPVE$	-37	-38	-25	-34	-41	-52

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

<sup>b</sup> Harmonic computations, SNSD basis set.

<sup>c</sup> Harmonic computations, 6-311++G(2d,2p) basis set

<sup>d</sup> Harmonic computations maug-cc-pVTZ basis set

 $^{\rm e}$  Hybrid model, harmonic part at B2PLYP/6-311++G(2d,2p) level and anharmonic corrections from B3LYP/SNSD computations.

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

			SF1a	SF1b	SF2a	SF2b	SF3a	SF3b
	$\Delta H$	RRHO	495.84	-0.01	0.02	-0.02	-0.08	-0.12
B2/B3	(kJ/mol)	HRAO <sup>b</sup>	491.15	0.02	-0.42	-0.42	0.17	0.03
	$\Delta S$	RRHO	424.5	-0.04	2.53	2.75	-4.19	-4.22
	(J/mol· K)	HRAO <sup>b</sup>	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 <sup>b</sup>	362.5	-0.07	-0.86	-0.5	1.29	1.17
	$\Delta H$	RRHO	496.21	-0.01	-0.01	-0.02	-0.09	-0.1
	(kJ/mol)	HRAO <sup>b</sup>	491.42	-0.04	0.08	-0.5	0.27	0.27
D2D2/D2D2	$\Delta S$	RRHO	423.39	0.64	2.68	5.39	-3.61	-3.84
B2D3/B3D3	(J/mol· K)	HRAO <sup>b</sup>	430.03	0.56	2.11	1.52	-4.38	-3.59
	ΔG	RRHO	369.98	-0.2	-0.81	-1.63	0.99	1.04
	(kJ/mol)	HRAO <sup>b</sup>	363.2	-0.21	-0.55	-0.95	1.57	1.34

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.

<sup>a</sup> Values with respect to the SF1a conformer. All thermodynamic properties have been computed at 298 K and 1 atm.

<sup>b</sup> The two lowest vibrations have been described by hindered-rotor contributions computed by means of an automatic procedure<sup>86</sup> 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)<sup>38</sup>, (see text for details).

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

	B3LYP <sup>b</sup>	B3LYP- D3 <sup>b</sup>	B3LYP- D3 <sup>c</sup>	B2PLYP <sup>d</sup>	B2PLYP- D3 <sup>d</sup>	B2PLYP- D3 <sup>e</sup>		CCSD(T) <sup>e</sup>	
	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 <sup> a</sup>
SF1b	0.04	0.06	0.06	0.19	0.19	0.06	0.06	$0.06^{\mathrm{f}}$	$0.06^{\rm f}$
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	$1.45^{ m f}$	$1.41^{ m f}$
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 <sup>f</sup>	$0.26^{\rm f}$

<sup>*a*</sup> 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.

<sup>b</sup> computed at B3LYP/SNSD optimized structure.

<sup>c</sup> computed at B3LYP-D3/SNSD optimized structure.

<sup>d</sup> computed at B2PLYP/6-311++G(2d,2p) optimized structure.

<sup>e</sup> computed at B2PLYP-D3/maug-cc-pVTZ optimized structure.

<sup>*f*</sup> difference between a and b conformers computed at the CCSD(T)/cc-pVTZ level.

	SF1a	SF1b	SF2a	SF2b	SF3a	SF3b
A <sub>0</sub> /MHz	2223.48	2209.77	2977.97	2886.53	2248.40	2219.00
B <sub>0</sub> /MHz	551.00	549.70	489.08	491.19	574.46	578.44
C <sub>0</sub> /MHz	457.31	457.13	433.76	438.37	519.91	523.44
μ <sub>a</sub> 298K/D	0.05	0.06	0.33	0.30	0.14	0.15
μ <sub>b</sub> 298K/D	-0.19	0.03	-0.17	0.06	-0.40	-0.09
μ <sub>c</sub> 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 S8. The best estimated vibrationally averaged rotational constants and dipole moment components  $(\boldsymbol{\mu})$  .

Table S9. Selected structural and energetic parameters of transition states<sup>a</sup>.

Transition	В	2PLYP					]	B2PLYP-D3				
States	ΔE	$\Delta E^{\#b}$	ΔE	ΔEZPVE	$\Delta E^{\#b}$	$\Delta EZPVE^{\#b}$	$\Delta G$	$\Delta G^{\#b}$	ν	$C_2C_3C_{10}C_{13}$	$C_{3}C_{10}C_{13}C_{15}$	$C_6C_5O_{18}C_{20}$
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;  $\Delta E$ , ZPVE corrected  $\Delta EZPVE$  and  $\Delta G$  at 298 K in kJ/mol are reported with respect to the SF1a conformer, wavenumber ( $\nu$ ) in cm<sup>-1</sup>, angles in degrees.

<sup>b</sup> 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

		1851-140	
	Х	Y	Z
С	1.034977	1.828040	0.155405
С	-0.362492	1.806074	-0.024999
С	-1.063872	0.620841	-0.259183
С	-0.369163	-0.607805	-0.314419
С	0.997934	-0.572741	-0.140022
С	1.686677	0.614650	0.090304
Н	1.572080	2.751945	0.337198
Н	-0.909740	2.743270	0.016943
Н	-0.893774	-1.543054	-0.479354
С	-2.567904	0.631558	-0.457280
Н	-2.922934	1.665511	-0.368601
Н	-2.815977	0.294100	-1.471668
С	-3.287243	-0.234592	0.540071
Н	-3.140256	0.023396	1.588609
С	-4.054339	-1.283155	0.222946
Н	-4.545140	-1.879032	0.985794
Н	-4.215425	-1.572077	-0.812854
0	1.880601	-1.627253	-0.154460
0	3.030566	0.356283	0.231064
C	3.179658	-1.063462	0.081409
Н	3.823909	-1.270359	-0.778039
Н	3.592525	-1.482382	1.003751
		tsSF2ab	
		toor atto	
	Х	Y	Z
С	X 0.464488	Y 1.632234	Z -0.141791
C C	X 0.464488 -0.820785	Y 1.632234 1.073090	Z -0.141791 -0.256875
C C C	X 0.464488 -0.820785 -1.032412	Y 1.632234 1.073090 -0.310338	Z -0.141791 -0.256875 -0.260004
C C C C	X 0.464488 -0.820785 -1.032412 0.064754	Y 1.632234 1.073090 -0.310338 -1.187290	Z -0.141791 -0.256875 -0.260004 -0.136595
C C C C C	X 0.464488 -0.820785 -1.032412 0.064754 1.321812	Y 1.632234 1.073090 -0.310338 -1.187290 -0.625885	Z -0.141791 -0.256875 -0.260004 -0.136595 -0.023277
C C C C C C	X 0.464488 -0.820785 -1.032412 0.064754 1.321812 1.519830	Y 1.632234 1.073090 -0.310338 -1.187290 -0.625885 0.749011	Z -0.141791 -0.256875 -0.260004 -0.136595 -0.023277 -0.026278
C C C C C C H	X 0.464488 -0.820785 -1.032412 0.064754 1.321812 1.519830 0.621002	Y 1.632234 1.073090 -0.310338 -1.187290 -0.625885 0.749011 2.705007	Z -0.141791 -0.256875 -0.260004 -0.136595 -0.023277 -0.026278 -0.140474
C C C C C H H	X 0.464488 -0.820785 -1.032412 0.064754 1.321812 1.519830 0.621002 -1.677095	Y 1.632234 1.073090 -0.310338 -1.187290 -0.625885 0.749011 2.705007 1.735327	Z -0.141791 -0.256875 -0.260004 -0.136595 -0.023277 -0.026278 -0.140474 -0.339769
С С С С С Н Н Н	X 0.464488 -0.820785 -1.032412 0.064754 1.321812 1.519830 0.621002 -1.677095 -0.070369	Y 1.632234 1.073090 -0.310338 -1.187290 -0.625885 0.749011 2.705007 1.735327 -2.263979	Z -0.141791 -0.256875 -0.260004 -0.136595 -0.023277 -0.026278 -0.140474 -0.339769 -0.132527
С С С С С С Н Н Н С	X 0.464488 -0.820785 -1.032412 0.064754 1.321812 1.519830 0.621002 -1.677095 -0.070369 -2.436460	Y 1.632234 1.073090 -0.310338 -1.187290 -0.625885 0.749011 2.705007 1.735327 -2.263979 -0.869310	Z -0.141791 -0.256875 -0.260004 -0.136595 -0.023277 -0.026278 -0.140474 -0.339769 -0.132527 -0.411559
С С С С С С Н Н Н С Н	X 0.464488 -0.820785 -1.032412 0.064754 1.321812 1.519830 0.621002 -1.677095 -0.070369 -2.436460 -2.799481	Y           1.632234           1.073090           -0.310338           -1.187290           -0.625885           0.749011           2.705007           1.735327           -2.263979           -0.869310           -0.699954	Z -0.141791 -0.256875 -0.260004 -0.136595 -0.023277 -0.026278 -0.140474 -0.339769 -0.132527 -0.411559 -1.433302
С С С С С С Н Н Н Н Н Н	X 0.464488 -0.820785 -1.032412 0.064754 1.321812 1.519830 0.621002 -1.677095 -0.070369 -2.436460 -2.799481 -2.395825	Y 1.632234 1.073090 -0.310338 -1.187290 -0.625885 0.749011 2.705007 1.735327 -2.263979 -0.869310 -0.699954 -1.956095	Z -0.141791 -0.256875 -0.260004 -0.136595 -0.023277 -0.026278 -0.140474 -0.339769 -0.132527 -0.411559 -1.433302 -0.267033
С С С С С С С Н Н Н С Н Н С Н	X 0.464488 -0.820785 -1.032412 0.064754 1.321812 1.519830 0.621002 -1.677095 -0.070369 -2.436460 -2.799481 -2.395825 -3.412037	Y           1.632234           1.073090           -0.310338           -1.187290           -0.625885           0.749011           2.705007           1.735327           -2.263979           -0.869310           -0.699954           -1.956095           -0.273082	Z -0.141791 -0.256875 -0.260004 -0.136595 -0.023277 -0.026278 -0.140474 -0.339769 -0.132527 -0.411559 -1.433302 -0.267033 0.564433
С С С С С С С Н Н Н С Н Н С Н Н	X 0.464488 -0.820785 -1.032412 0.064754 1.321812 1.519830 0.621002 -1.677095 -0.070369 -2.436460 -2.799481 -2.395825 -3.412037 -3.171374	Y           1.632234           1.073090           -0.310338           -1.187290           -0.625885           0.749011           2.705007           1.735327           -2.263979           -0.669910           -0.699954           -1.956095           -0.273082           -0.403554	Z -0.141791 -0.256875 -0.260004 -0.136595 -0.023277 -0.026278 -0.140474 -0.339769 -0.132527 -0.411559 -1.433302 -0.267033 0.564433 1.619206
С С С С С С С С С Н Н Н С Н Н С Н С С	X 0.464488 -0.820785 -1.032412 0.064754 1.321812 1.519830 0.621002 -1.677095 -0.070369 -2.436460 -2.799481 -2.395825 -3.412037 -3.171374 -4.513971	Y           1.632234           1.073090           -0.310338           -1.187290           -0.625885           0.749011           2.705007           1.735327           -2.263979           -0.669910           -0.699954           -1.956095           -0.273082           -0.403554           0.402436	Z -0.141791 -0.256875 -0.260004 -0.136595 -0.023277 -0.026278 -0.140474 -0.339769 -0.132527 -0.411559 -1.433302 -0.267033 0.564433 1.619206 0.221180
С С С С С С С С С Н Н Н С Н Н С Н С Н Н С Н Н С	X 0.464488 -0.820785 -1.032412 0.064754 1.321812 1.519830 0.621002 -1.677095 -0.070369 -2.436460 -2.799481 -2.395825 -3.412037 -3.171374 -4.513971 -5.183261	Y           1.632234           1.073090           -0.310338           -1.187290           -0.625885           0.749011           2.705007           1.735327           -2.263979           -0.669910           -0.699954           -1.956095           -0.273082           -0.403554           0.402436           0.814805	Z -0.141791 -0.256875 -0.260004 -0.136595 -0.023277 -0.026278 -0.140474 -0.339769 -0.132527 -0.411559 -1.433302 -0.267033 0.564433 1.619206 0.221180 0.969456
С С С С С С С С С С Н Н Н С Н Н С Н Н Н С Н Н Н Н С	X 0.464488 -0.820785 -1.032412 0.064754 1.321812 1.519830 0.621002 -1.677095 -0.070369 -2.436460 -2.799481 -2.395825 -3.412037 -3.171374 -4.513971 -5.183261 -4.778385	Y           1.632234           1.073090           -0.310338           -1.187290           -0.625885           0.749011           2.705007           1.735327           -2.263979           -0.669910           -0.699954           -1.956095           -0.273082           -0.403554           0.402436           0.814805           0.558451	Z -0.141791 -0.256875 -0.260004 -0.136595 -0.023277 -0.026278 -0.140474 -0.339769 -0.132527 -0.411559 -1.433302 -0.267033 0.564433 1.619206 0.221180 0.969456 -0.821869
С С С С С С С С С С С С С С С С С С С	X 0.464488 -0.820785 -1.032412 0.064754 1.321812 1.519830 0.621002 -1.677095 -0.070369 -2.436460 -2.799481 -2.395825 -3.412037 -3.171374 -4.513971 -5.183261 -4.778385 2.528870	Y           1.632234           1.073090           -0.310338           -1.187290           -0.625885           0.749011           2.705007           1.735327           -2.263979           -0.869310           -0.699954           -1.956095           -0.273082           -0.403554           0.402436           0.814805           0.558451           -1.272120	Z -0.141791 -0.256875 -0.260004 -0.136595 -0.023277 -0.026278 -0.140474 -0.339769 -0.132527 -0.411559 -1.433302 -0.267033 0.564433 1.619206 0.221180 0.969456 -0.821869 0.108336
С С С С С С С С С С С С С С С С С С С	X 0.464488 -0.820785 -1.032412 0.064754 1.321812 1.519830 0.621002 -1.677095 -0.070369 -2.436460 -2.799481 -2.395825 -3.412037 -3.171374 -4.513971 -5.183261 -4.778385 2.528870 2.861045	Y           1.632234           1.073090           -0.310338           -1.187290           -0.625885           0.749011           2.705007           1.735327           -2.263979           -0.869310           -0.699954           -1.956095           -0.273082           -0.403554           0.402436           0.814805           0.558451           -1.272120           1.029673	Z -0.141791 -0.256875 -0.260004 -0.136595 -0.023277 -0.026278 -0.140474 -0.339769 -0.132527 -0.411559 -1.433302 -0.267033 0.564433 1.619206 0.221180 0.969456 -0.821869 0.108336 0.103131
С С С С С С С С С С С С С С С С С С С	X 0.464488 -0.820785 -1.032412 0.064754 1.321812 1.519830 0.621002 -1.677095 -0.070369 -2.436460 -2.799481 -2.395825 -3.412037 -3.171374 -4.513971 -5.183261 -4.778385 2.528870 2.861045 3.524192	Y           1.632234           1.073090           -0.310338           -1.187290           -0.625885           0.749011           2.705007           1.735327           -2.263979           -0.869310           -0.699954           -1.956095           -0.273082           -0.403554           0.402436           0.814805           0.558451           -1.272120           1.029673           -0.240005	Z -0.141791 -0.256875 -0.260004 -0.136595 -0.023277 -0.026278 -0.140474 -0.339769 -0.132527 -0.411559 -1.433302 -0.267033 0.564433 1.619206 0.221180 0.969456 -0.821869 0.108336 0.103131 0.193802
С С С С С С С С С С С С С С С С С С С	X 0.464488 -0.820785 -1.032412 0.064754 1.321812 1.519830 0.621002 -1.677095 -0.070369 -2.436460 -2.799481 -2.395825 -3.412037 -3.171374 -4.513971 -5.183261 -4.778385 2.528870 2.861045 3.524192 4.222837	Y           1.632234           1.073090           -0.310338           -1.187290           -0.625885           0.749011           2.705007           1.735327           -2.263979           -0.869310           -0.699954           -1.956095           -0.273082           -0.403554           0.402436           0.814805           0.558451           -1.272120           1.029673           -0.240005           -0.343329	Z -0.141791 -0.256875 -0.260004 -0.136595 -0.023277 -0.026278 -0.140474 -0.339769 -0.132527 -0.411559 -1.433302 -0.267033 0.564433 1.619206 0.221180 0.969456 -0.821869 0.108336 0.103131 0.193802 -0.641512

		tsSF3ab	
	Х	Y	Z
С	0.614187	1.772889	0.191496
С	-0.722935	1.534107	-0.179454
С	-1.169851	0.272870	-0.583471
С	-0.265585	-0.809938	-0.629448
С	1.041947	-0.564472	-0.263666
С	1.474152	0.695107	0.137563
H	0.954004	2.754815	0.500496
H	-1.430530	2.357434	-0.147229
H C	-0.58/368	-1./99/43	-0.936461
с н	-2.019242	0.048970	-0.937108
н	-2.692250	-0 665032	-1.313270
C	-3 477390	-0.454813	0 199827
н	-4.519411	-0.644169	-0.057879
C	-3.070403	-0.674628	1.454073
Ĥ	-3.761610	-1.035796	2.208670
н	-2.043000	-0.500064	1.758555
0	2.093825	-1.450166	-0.233225
0	2.816417	0.655687	0.437613
С	3.235570	-0.697145	0.204187
Н	3.997470	-0.708818	-0.580794
Н	3.613055	-1.124486	1.137609
		tsSF12a	
C	X	Y	Z
C	-0.890324	1./869/6	-0.16/801
C C	0.4/8455	1.012912	0.1101/8
c	0 200401	-0 784929	0.377234
C	-1.138860	-0.602574	0.129169
C	-1.674681	0.652837	-0.150519
Ĥ	-1.306707	2.762710	-0.390857
Н	1.127078	2.483991	0.117846
н	0.601362	-1.771003	0.616696
С	2.506309	0.205172	0.670689
Н	2.936660	1.187051	0.897240
Н	2.649056	-0.408153	1.569495
С	3.263591	-0.424548	-0.484851
Н	2.669287	-0.706826	-1.352465
С	4.582738	-0.642370	-0.498317
H	5.069973	-1.093769	-1.356315
Н	5.214921	-0.375516	0.345478
0	-2.129896	-1.554828	0.036651
U C	-3.018664	0.526614	-0.431046
с и	-3.349290	-0.802093	-0.010503
н	-4 025280	-0.704149	-0 735184
11	1.025200	tsSF12b	0.755104
	Х	Y	Z
С	0.881160	1.786074	0.176372
С	-0.490037	1.608367	-0.092423
С	-1.030945	0.361145	-0.417723
С	-0.191233	-0.772338	-0.484287
С	1.148486	-0.588567	-0.211641
С	1.675223	0.660254	0.111522
Н	1.293655	2.759377	0.416649
Н	-1.148878	2.470348	-0.042720
Н	-0.582970	-1.750495	-0.744891
C	-2.513326	0.200077	-0.659189
H U	-2.952048	1.1/9543	-0.880394
п С	-2.0/1103	-0.41/322	-1.332302
с и	-3.244821	-0.42/813	0.313939
п С	-2.032343 -4 561813	-0.700328	0 552820
н	-5.029818	-1.105640	1.422184
н	-5.211280	-0.398712	-0.280858
0	2.165885	-1.516002	-0.261091
0	3.040413	0.555018	0.273073
С	3.284291	-0.854607	0.344952
Н	3.352440	-1.156356	1.398608
Н	4.190346	-1.094325	-0.210109

		tsSF13a	
	Х	Y	Z
С	0.690142	1.773167	0.302592
С	-0.647666	1.587437	-0.089626
С	-1.129134	0.352780	-0.539879
С	-0.257009	-0.752509	-0.619834
С	1.055038	-0.558086	-0.234743
С	1.519892	0.673006	0.216802
Н	1.053431	2.732223	0.654086
Н	-1.328946	2.432082	-0.041104
Η	-0.599697	-1.719186	-0.973846
С	-2.589775	0.189485	-0.905285
Н	-2.941718	1.098615	-1.402185
Н	-2.689753	-0.622635	-1.634758
С	-3.477659	-0.097980	0.294193
Н	-4.248901	0.637249	0.516768
С	-3.368067	-1.173196	1.080982
Н	-4.030306	-1.320528	1.927794
Н	-2.607058	-1.931001	0.912125
0	2.076588	-1.481526	-0.185151
0	2.848894	0.562256	0.569327
С	3.258719	-0.697123	0.023937
Н	3.753452	-0.528885	-0.941986
Н	3.908759	-1.205674	0.734862
		tsSF13b	
	Х	Y	Z
С	0.697763	1.777084	0.330902
С	-0.649028	1.604117	-0.035438
С	-1.137333	0.390551	-0.533248
С	-0.263309	-0.704833	-0.691125
С	1.054668	-0.526884	-0.319100
С	1.526363	0.682921	0.181371
Н	1.069934	2.724128	0.704958
Н	-1.333340	2.440114	0.077448
Н -0.608586		-1.650049	-1.096886
С -2.607734		0.235089	-0.859588
Н -2.982971		1.169512	-1.287670
Н	-2.725515	-0.532084	-1.633815
С	-3.452927	-0.133933	0.348439
Н	-4.223383	0.577829	0.639506
С	-3.307708	-1.252967	1.065288
Н	-3.940816	-1.458216	1.922274
Н	-2.545801	-1.990805	0.826568
0	2.100020	-1.418583	-0.424947
0	2.884453	0.590104	0.404352
C	3.161790	-0.812666	0.324444
н	3 173629	-1 236994	1 337351
Н	4.105804	-0.966485	-0.196646
		tsSF23a	
	Х	Y	Z
С	0.651437	1.770342	-0.004946
<u> </u>	-0.678665	1.477538	-0.366923
c			
C C	-1.117852	0.171479	-0.600245
C C C	-1.117852 -0.212581	0.171479 -0.905797	-0.600245 -0.479687
C C C C	-1.117852 -0.212581 1.087294	0.171479 -0.905797 -0.607273	-0.600245 -0.479687 -0.130840
C C C C C	-1.117852 -0.212581 1.087294 1.512626	0.171479 -0.905797 -0.607273 0.699250	-0.600245 -0.479687 -0.130840 0.102985
C C C C H	-1.117852 -0.212581 1.087294 1.512626 0.981632	0.171479 -0.905797 -0.607273 0.699250 2.786375	-0.600245 -0.479687 -0.130840 0.102985 0.179188
С С С С Н Н	-1.117852 -0.212581 1.087294 1.512626 0.981632 -1.383589	0.171479 -0.905797 -0.607273 0.699250 2.786375 2.296805	-0.600245 -0.479687 -0.130840 0.102985 0.179188 -0.473428
С С С С Н Н Н	-1.117852 -0.212581 1.087294 1.512626 0.981632 -1.383589 -0.527374	0.171479 -0.905797 -0.607273 0.699250 2.786375 2.296805 -1.930680	-0.600245 -0.479687 -0.130840 0.102985 0.179188 -0.473428 -0.647587
С С С С С С Н Н Н С	-1.117852 -0.212581 1.087294 1.512626 0.981632 -1.383589 -0.527374 -2.564209	0.171479 -0.905797 -0.607273 0.699250 2.786375 2.296805 -1.930680 -0.105161	-0.600245 -0.479687 -0.130840 0.102985 0.179188 -0.473428 -0.647587 -0.954102
С С С С С С С С Н Н Н С Н	-1.117852 -0.212581 1.087294 1.512626 0.981632 -1.383589 -0.527374 -2.564209 -3.040628	0.171479 -0.905797 -0.607273 0.699250 2.786375 2.296805 -1.930680 -0.105161 0.834467	-0.600245 -0.479687 -0.130840 0.102985 0.179188 -0.473428 -0.647587 -0.954102 -1.254952
ССССС ССС Н Н С Н	-1.117852 -0.212581 1.087294 1.512626 0.981632 -1.383589 -0.527374 -2.564209 -3.040628 -2.607215	0.171479 -0.905797 -0.607273 0.699250 2.786375 2.296805 -1.930680 -0.105161 0.834467 -0.768484	-0.600245 -0.479687 -0.130840 0.102985 0.179188 -0.473428 -0.647587 -0.954102 -1.254952 -1.824440
ССССС ССС Н Н С Н С	-1.117852 -0.212581 1.087294 1.512626 0.981632 -1.383589 -0.527374 -2.564209 -3.040628 -2.607215 -3.349965	0.171479 -0.905797 -0.607273 0.699250 2.786375 2.296805 -1.930680 -0.105161 0.834467 -0.768484 -0.727684	-0.600245 -0.479687 -0.130840 0.102985 0.179188 -0.473428 -0.647587 -0.954102 -1.254952 -1.824440 0.187243
сссс СССС Н Н Н С Н	-1.117852 -0.212581 1.087294 1.512626 0.981632 -1.383589 -0.527374 -2.564209 -3.040628 -2.607215 -3.349965 -3.727789	0.171479 -0.905797 -0.607273 0.699250 2.786375 2.296805 -1.930680 -0.105161 0.834467 -0.768484 -0.727684 -1.736869	-0.600245 -0.479687 -0.130840 0.102985 0.179188 -0.473428 -0.647587 -0.954102 -1.254952 -1.824440 0.187243 0.033207
сссссни нсноси	-1.117852 -0.212581 1.087294 1.512626 0.981632 -1.383589 -0.527374 -2.564209 -3.040628 -2.607215 -3.349965 -3.727789 -3.593404	0.171479 -0.905797 -0.607273 0.699250 2.786375 2.296805 -1.930680 -0.105161 0.834467 -0.768484 -0.727684 -1.736869 -0.117807	-0.600245 -0.479687 -0.130840 0.102985 0.179188 -0.473428 -0.647587 -0.954102 -1.254952 -1.824440 0.187243 0.033207 1.351658
ССССНННСНС СССННС СССНС СССС СССС СССС	-1.117852 -0.212581 1.087294 1.512626 0.981632 -1.383589 -0.527374 -2.564209 -3.040628 -2.607215 -3.349965 -3.727789 -3.593404 -4.157095	0.171479 -0.905797 -0.607273 0.699250 2.786375 2.296805 -1.930680 -0.105161 0.834467 -0.768484 -0.727684 -1.736869 -0.117807 -0.607948	-0.600245 -0.479687 -0.130840 0.102985 0.179188 -0.473428 -0.647587 -0.954102 -1.254952 -1.824440 0.187243 0.033207 1.351658 2.138686
ССССНННСННСН НКСИНСИ	-1.117852 -0.212581 1.087294 1.512626 0.981632 -1.383589 -0.527374 -2.564209 -3.040628 -2.607215 -3.349965 -3.727789 -3.593404 -4.157095 -3.225426	0.171479 -0.905797 -0.607273 0.699250 2.786375 2.296805 -1.930680 -0.105161 0.834467 -0.768484 -0.727684 -1.736869 -0.117807 -0.607948 0.884816	-0.600245 -0.479687 -0.130840 0.102985 0.179188 -0.473428 -0.647587 -0.954102 -1.254952 -1.824440 0.187243 0.033207 1.351658 2.138686 1.556249
ССССНННСНСНСННО	-1.117852 -0.212581 1.087294 1.512626 0.981632 -1.383589 -0.527374 -2.564209 -3.040628 -2.607215 -3.349965 -3.727789 -3.593404 -4.157095 -3.225426 2.134521	0.171479 -0.905797 -0.607273 0.699250 2.786375 2.296805 -1.930680 -0.105161 0.834467 -0.768484 -0.727684 -1.736869 -0.117807 -0.607948 0.884816 -1.475586	-0.600245 -0.479687 -0.130840 0.102985 0.179188 -0.473428 -0.647587 -0.954102 -1.254952 -1.824440 0.187243 0.033207 1.351658 2.138686 1.556249 0.086947
ССССНННСНСНСННО ОО	-1.117852 -0.212581 1.087294 1.512626 0.981632 -1.383589 -0.527374 -2.564209 -3.040628 -2.607215 -3.349965 -3.727789 -3.593404 -4.157095 -3.225426 2.134521 2.839456	0.171479 -0.905797 -0.607273 0.699250 2.786375 2.296805 -1.930680 -0.105161 0.834467 -0.768484 -0.727684 -1.736869 -0.117807 -0.607948 0.884816 -1.475586 0.690174	-0.600245 -0.479687 -0.130840 0.102985 0.179188 -0.473428 -0.647587 -0.954102 -1.254952 -1.824440 0.187243 0.033207 1.351658 2.138686 1.556249 0.086947 0.478339
ССССНННСНСНСННООС	-1.117852 -0.212581 1.087294 1.512626 0.981632 -1.383589 -0.527374 -2.564209 -3.040628 -2.607215 -3.349965 -3.727789 -3.593404 -4.157095 -3.225426 2.134521 2.839456 3.291270	0.171479 -0.905797 -0.607273 0.699250 2.786375 2.296805 -1.930680 -0.105161 0.834467 -0.768484 -0.727684 -1.736869 -0.117807 -0.607948 0.884816 -1.475586 0.690174 -0.632402	-0.600245 -0.479687 -0.130840 0.102985 0.179188 -0.473428 -0.647587 -0.954102 -1.254952 -1.824440 0.187243 0.033207 1.351658 2.138686 1.556249 0.086947 0.478339 0.165183
ССССНННСНСННООСН	-1.117852 -0.212581 1.087294 1.512626 0.981632 -1.383589 -0.527374 -2.564209 -3.040628 -2.607215 -3.349965 -3.727789 -3.593404 -4.157095 -3.225426 2.134521 2.839456 3.291270 3.794433	0.171479 -0.905797 -0.607273 0.699250 2.786375 2.296805 -1.930680 -0.105161 0.834467 -0.768484 -0.727684 -1.736869 -0.117807 -0.607948 0.884816 -1.475586 0.690174 -0.632402 -0.620826	-0.600245 -0.479687 -0.130840 0.102985 0.179188 -0.473428 -0.647587 -0.954102 -1.254952 -1.824440 0.187243 0.033207 1.351658 2.138686 1.556249 0.086947 0.478339 0.165183 -0.810852

		tsSF23b	
	Х	Y	Z
С	0.642386	1.771658	-0.003003
С	-0.692684	1.477675	-0.344317
С	-1.124257	0.175775	-0.613485
С	-0.205507	-0.894975	-0.554476
С	1.096605	-0.596684	-0.213614
С	1.513957	0.705086	0.058200
Н	0.970407	2.786035	0.193758
Н	-1.409252	2.291862	-0.399932
Н	-0.510813	-1.914423	-0.767173
С	-2.577831	-0.105246	-0.931177
Н	-3.065898	0.833211	-1.216736
Н	-2.639842	-0.766499	-1.801882
С	-3.331504	-0.734650	0.228089
Н	-3.712230	-1.743403	0.078323
С	-3.543852	-0.132275	1.402469
Н	-4.085707	-0.628028	2.201239
Н	-3.171773	0.869553	1.603397
0	2.176750	-1.448714	-0.137581
0	2.869558	0.709232	0.310864
С	3.202466	-0.671677	0.494193
Н	4.159394	-0.879977	0.017335
Н	3.216573	-0.900612	1.568130

Table S11. Infrared frequencies and intensities of SF	, SF2 and SF3 in xenon matric	es and their tentative assignment
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B2PLYP-D3/B3LYP-D3		Emocioo	Xe(30K/11K)		()		
$\nu_{anh}/cm^{\text{-}1}$	I/km mol <sup>-1</sup>	mode	Species	$\nu/cm^{-1}$	band	I <sup>a</sup>	Approximate Description"
3106	17	60	SF3	3074		vw	$v_{as} = CH_2$
3099	2	59	SF1	n.o.			vCH(R)
3098	18	60	SF1	3085		vw	$v_{as}$ =CH <sub>2</sub>
3098	19	60	SF2	3063		vw	v <sub>as</sub> =CH <sub>2</sub>
3094	5	59	SF2	n.o.			vCH(R)
3094	4	59	SF3	n.o.			vCH(R)
3072	3	57	SF2	n.o.			vCH(R)
3069	9	57	SF1	3080		vw	vCH(R)
3064	5	58	SF3	n.o.			vCH(R)
3063	5	58	SF2	3042		vw	vCH(R)
3063	3	58	SF1	n.o.			vCH(R)
3051	9	57	SF3	n.o.			vCH(R)
3026	9	56	SF3	n.o.			$v_s = CH_2 + vCH$
3023	6	56	SF1	3034		vw	$v_s = CH_2 + vCH$
3023	6	56	SF2	n.o.			$v_{e} = CH_{2} + vCH$
3005	48	54	SF3	2979		sh.vw	$v_{ac}$ CH <sub>2</sub> (OX)
3002	30	55	SF3	n o		,	vCH
3002	45	54	SF2	2991		vw	v <sub>ec</sub> CH <sub>2</sub> (OX)
2999	14	55	SF1	2984		VW	vCH
2999	16	55	SF2	3009		vw	vCH
2988	43	54	SF1	2965		VW	v <sub></sub> CH <sub>2</sub> (OX)
2968	68	45+47	SF3	2953		NNN	vas on 2001
2942	22	52	SF2	2968		sh vw	v-CH <sub>2</sub>
2938	14	53	SF1	2918			v CH <sub>2</sub>
2936	6	52	SF3	2910		***	v CH <sub>2</sub>
2930	13	53	SE2	2895		vw	v CH-
2933	13	53	SF2	2003			v <sub>as</sub> err <sub>2</sub>
2910	67	51	SE2	2903		ch w	
2892	07	51	SF2 SE1	2879		sii,w	$v C_{20} H_{21}$
2091	93	51	51-1	2012		w	
2890	58	51	SF3	2874		w	$VC_{20}H_{21}$
2871	24	52	SF1	2881		sh,vw	v <sub>s</sub> CH <sub>2</sub>
2745-2780	2	over+combi	SF1	2773		vw	
2740-2790	2	over+combi	SF2	2768		vw	
1665	1	49	SF2	n.o.			$vCC(R)+\delta CCC(R)$
1660	2 (20)	50	SF1	1646		vw	vC=C+s=CH
1660	14	50	SF2	1645		sh,vw	vC=C+s=CH <sub>2</sub>
1659	10	50	SF3	1639		vw	vC=C+s=CH <sub>2</sub>
1635	1 (2)	49	SF1	n.o.			$vCC(R)+\delta CCC(R)$
1635	1 (3)	49	SF3	n.o.			$vCC(R)+\delta CCC(R)$
1620-1635	4	over+combi		1618		vw	
1614	2 (6)	48	SF1	1612		vw	$vCC(R)+\delta CCC(R)$
1610	4	48	SF3	1609		vw	$\nu CC(R) + \delta CCC(R)$
1609	6	48	SF2	1605		vw	$\nu CC(R) + \delta CCC(R)$
1519	9 (31)	47	SF2	1514		vw	s-CH <sub>2</sub> (OX)
1516	25 (31)	47	SF1	1510		vw	s-CH <sub>2</sub> (OX)
1516 (1510)	8 (47)	47	SF3	1507		sh, vw	s-CH <sub>2</sub> (OX)
1493 (1496)	17 (145)	46	SF3	1502		sh, m	$\delta$ CCH(R)+ $\nu$ CC(R)+s-CH <sub>2</sub> (OX)
1494	160	46	SF2	1501		s	$\delta$ CCH(R)+vCC(R)+s-CH <sub>2</sub> (OX)
1493	75 (90)	46	SF1	1489		vs	$\delta$ CCH(R)+vCC(R)+s-CH <sub>2</sub> (OX)

1456	24 (52)	44	SF2	1445		sh, w	$s{=}CH_2{+}\nu CC(R){+}\delta CCC(R){+}t{-}CH_2{+}\omega{-}CH_2(OX)$
1457 (1454)	8 (98)	44	SF1	1444		S	$s=CH_2+\nu CC(R)+\delta CCC(R)+t\text{-}CH_2+\omega-CH_2(OX)$
1452	14	44	SF3	1447		sh, w	s-CH <sub>2</sub>
1448	63 (85)	45	SF3	1447		sh, w	$s=CH_2+\nu CC(R)+\delta CCC(R)+t-CH_2+\omega-CH_2(OX)$
1447	23	45	SF2	1430		sh, vw	s-CH <sub>2</sub>
1443	10	45	SF1	1432		vw	s-CH <sub>2</sub>
1429	1 (4)	43	SF1	n.o.			$s=CH_2+\delta CH+s-CH_2$
1429	1	43	SF2	n.o.			$s=CH_2+\delta CH+s-CH_2$
1421	3 (5)	43	SF3	1434		vw	s=CH <sub>2</sub> +δCH+s-CH <sub>2</sub>
1412	1	42	SF2	n.o.			$\omega$ -CH <sub>2</sub> (OX)
1407 (1409)	1 (5)	42	SF3	1405		vvw	$\omega$ -CH <sub>2</sub> (OX)
1406 (1398)	1 (4)	42	SF1	1409		vvw	$\omega$ -CH <sub>2</sub> (OX)
1383	5	14+11	SF2	1397		vvw	
1380	8	41	SF1	1363		vw	δCH+t-CH <sub>2</sub>
1379	7	41	SF3	1354		vw	t-CH <sub>2</sub> + $\nu$ CC(R)+ $\delta$ CCH(R)
1376 (1367)	2(7)	41	SF2	1362		vw	t-CH <sub>2</sub> + $\nu$ CC(R)+ $\delta$ CCH(R)
1331	3	40	SF3	n.o.			ω-CH <sub>2</sub> +δCH+δCCH(R)
1310	1 (13)	40	SF2	n.o.		vw	δCH+t-CH <sub>2</sub>
1309	1	40	SF1	n.o.			ω-CH <sub>2</sub> +δCH+δCCH(R)
1299 (1301)	1 (5)	39	SF1	1300		vw	t-CH <sub>2</sub> + $\nu$ CC(R)+ $\delta$ CCH(R)
1301	2	39	SF3	n.o.		vw	δCH+t-CH <sub>2</sub>
1295	17 (24)	39	SF2	1287		vw	ω-CH <sub>2</sub> +δCH+δCCH(R)
1293	11	38	SF3	1273		vw	t-CH <sub>3</sub> +δCH(R)
1278	15	15+14	SF1	1268	А	vw	
1276	5 (95)	38	SF2	1268	A	vw	t-CH <sub>a</sub> +\deltaCH(R)
1201 (1270)	22 (44)	38	SF1	1248	B	w	t-CH <sub>2</sub> +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	$vCC(R)+t-CH_2$
1258	39 (48)	37	SF3	n.o	C		$vCC(R)+t-CH_2$
1257	135 (156)	37	SF1	1231	C	sh w	vCC(R)+t-CH <sub>2</sub>
1249	12 (18)	32+3	SF3	n o	C	511, 17	
1237	3	4+31	SF1	n.o.	C		
1212 (1225)	1 (17)	36	SF1	1224	D	w	t-CH <sub>2</sub> +vCC(R)+vCO
1216	18 (31)	36	SF2	1221	D	w	$t-CH_2+\nu CC(R)+\nu CO$
1204	15 (18)	36	SF3	1196	E	vw	$t-CH_2(OX)+vCC(R)+vCO$
1203	4 (10)	35	SF2	1203	Ē	vw	$t-CH_2(OX)+vCC(R)+vCO$
1200	9	35	SF1	n o	Ľ		$t-CH_2(QX)+vCC(R)+vCQ$
1189	1 (17)	35	SF3	1183	F	VW	$t-CH_2+vCC(R)+vCO$
1184	9	34	SF2	1175	F	sh vw	$t-CH_2(OX)+\delta CH(R)+\delta CH+vCC(R)+vCO$
1183	9 (20)	34	SF1	1174	F		$t-CH_{2}(OX)+\delta CH(R)+\delta CH+vCC(R)+vCO$
1182	2	34	SF3	1174	F	VW	$t-CH_2(OX)+\delta CH(R)+\delta CH+vCC(R)+vCO$
1139	~ 0	32	SF3	1127	•	VW	$r-CH_2(OX)+\delta CH(R)$
1137	7	32	SF2	1127	N	vw	$r-CH_2(OX)+\delta CH(R)$
1137	12	33	SF1	1133	N	VW	$\delta CH(R)+r-CH_2(OX)$
1131	12	33	SF2	1130	N	VW	$\delta CH(R) + r - CH_2(OX)$
1127	6	33	SF3	1122	1	VW	$\delta CH(R) + r - CH_2(OX)$
1127	10	32	SF1	1122	0	VW	r-CH <sub>2</sub> (OX)+δCH(R)
1111	3 (6)	31	SF1	1120	P	VVV	$s_{-}CH_{2}(OH) + OCH(R)$
1107	2	31	SF2	1117	ı D	V W	s-CH <sub>2</sub> +δCH+vCC(R)
1107	1	12+14	SF1	1098	0	v vv	
1105	1 0	31	SF3	1101	Y	V VV	$\delta CH(R) + \delta CH + v CC(R) + v CO$
100	2 8	30	SE2	1001	0	v W	
1099	8 (12)	30	SF1	1091	v O	V W	
1027	2	7,10	SF1 SF1	1004	V O	v W	UCH(K)TUCH+VCC(K)+VCU
1093	3	7+19	511	1094	Q	vW	I

1061	1	30	SF3	n.o.			r=CH₂+δCH
1043 (1048)	48 (134)	29	SF2	1044		vs	νCO+δCH
1044	113	29	SF1	1044		vs	$\nu CO+\delta CH$
1043	96	29	SF3	1044		vs	νCO+δCH
1015	17	28	SF2	1024		vw	$\gamma CH+t=CH_2$
1015	18	28	SF1	998		vw	$\gamma CH+t=CH_2$
1016	10	28	SF3	993		vw	$\gamma CH+t=CH_2$
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	$\gamma CH+r-CH_2$
951	10	8+13	SF1	n.o.			
946	2(4)	11+12	SF2	946	Н	sh, vw	
942	3 (37)	25	SF3	938	Н	vw	$vCO+\gamma CH+\omega=CH_2$
941	5	11+12	SF1	n.o.			
939	10 (49)	26	SF1	944	Н	w	$\nu CO + \gamma CH + \omega = CH_2$
938(939)	19 (49)	25	SF1	944	Н	w	ω=CH <sub>2</sub>
936	37 (87)	24	SF2	946	Н	w	$\nu CO+\gamma CH+\omega=CH_2$
935	13	5+17	SF3	928	Ι	vw	
933	9	27	SF1	925	Ι	vw	$\gamma CH+r-CH_2+\nu CC+\nu CO$
930	12	23	SF1	915	J	m	$\delta CCC+\gamma CH+\omega=CH_2$
927(926)	54 (87)	26	SF2	915	J	sh, m	$\omega = CH_2$
927	9 (46)	23	SF3	911	J	vw	vCC+vCO+r-CH <sub>2</sub>
926(927)	37 (46)	26	SF3	911	J	vw	$\omega = CH_2$
925(926)	2 (87)	25	SF2	915	J	sh, m	$\gamma CH(R) + \omega = CH_2$
918	1	24	SF3	908	K	vw	γCH(R)
916	9	24	SF1	907	K	w	$\gamma CH(R) + \omega = CH_2$
914	6	23	SF2	906	K	vw	$ω = CH_2 + ω - CH_2 + γCH$
909	10	22	SF2	902	L	vw	r=CH <sub>2</sub> +r-CH <sub>2</sub> +γCH
907	8	22	SF1	903	L	vw	r=CH <sub>2</sub> +r-CH <sub>2</sub> +γCH
900	1	22	SF3	900	L	vw	νCC+νCO+γCH
879	10	3+18	SF3	868	M	vw	CI
869	11	21	SF3	856	M	vw	γCH
869	12	21	SFI	847	M	vw	γCH
858	10	21	SF2	848	M	vw	γCH
821	10	20	51	810	R	vw ab any	
821	14	19	SF2	810	ĸ	sn, vw	VCC(R)+VCO
820 814	10	5,14	SF5 SF1	800	e	vw	VCC(R)+VCO
014	1	3+14	SF1 CE2	804	5	vw	-CCCC(P) to CH
812	12	20	SF2	804	2	vw	
811	12	20	SF3 8E2	//0 801	т	VW	ttttt(K)+yth
807	21	4+15	SF2	707	т	sii, vw	TCCCC(P) InCH
701	21	19	SF1	777	1	w	
/81	8(17)	18	SFI	776		vw	VCC(R)+VCO+0CCC
780	3	18	SF2	770		vw	VCC(R)+VCO+oCCC
769	10	18	SF3	772		vw	-CCCC(R)
744	1	17	3F3 SE2	705		vw	
740	1	17	SF2	n.o.			TCCCC(R)
720	4	17	SF1 SF1	721			8000 ( 8000 ( R)
720	2	16	SF1 SF2	721		vw	8COC+8CCC(R)
719	3	16	SF2	720		vw	8COC + 8CCC(R)
675	4	10	SF2	667		v w	$t = CH_{+} + \gamma CH_{+} + \delta CCC(R) + \tau CCCC(R)$
670	0 7(8)	15	SF2 SF1	666		vw	$t = CH_2 + \gamma CH + \delta CCC(R) + \tau CCCC(R)$
664	2 2	15	SE3	660		V VV	$\omega = CH_2 + \gamma CH + \delta CCC(R) + \tau CCCC(R)$
610	6	14	SF1	n o		v VV	$\tau CCCC(R) + \delta CCC(R) + t = CH_+ + vCH$
609	3	14	SF3	n.o.			τCCCC(R)+δCCC(R)+t=CH <sub>2</sub> +γCH
604	6	14	SF2	598		vw	τCCCC(R)+δCCC(R)+t=CH <sub>2</sub> +νCH
599	12	13	SF2	585		vw	t=CH <sub>2</sub> +vCH
594	8	13	SF1	584		sh. vw	t=CH <sub>2</sub> +γCH
564	11	13	SF3	554		vw	t=CH <sub>2</sub> +γCH
	-						

<sup>a</sup> Intensity: vs-very strong, s-strong, m-medium, w-weak, vw-very weak, sh-shoulder <sup>b</sup>Abbreviations: v - bond stretching,  $\delta$  - bending, deformation in plane,  $\gamma$  - out-of-plane bending,  $\tau$  - torsion, s – scissoring, r – rocking,  $\omega$  - wagging, t – twisting, R – phenolic ring, OX-1,3-dioxolane ring.