

# Conformational preference of a chiral terpene: Vibrational Circular Dichroism (VCD), Infrared and Raman study of S-(-)-limonene oxide.

*Juan Ramón Avilés Moreno, Francisco Partal Ureña and Juan Jesús López González\*.*

University of Jaén, Department of Physical and Analytical Chemistry. Campus Las Lagunillas, E-23071  
Jaén (Spain).

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\*To whom correspondence should be addressed. Present address:

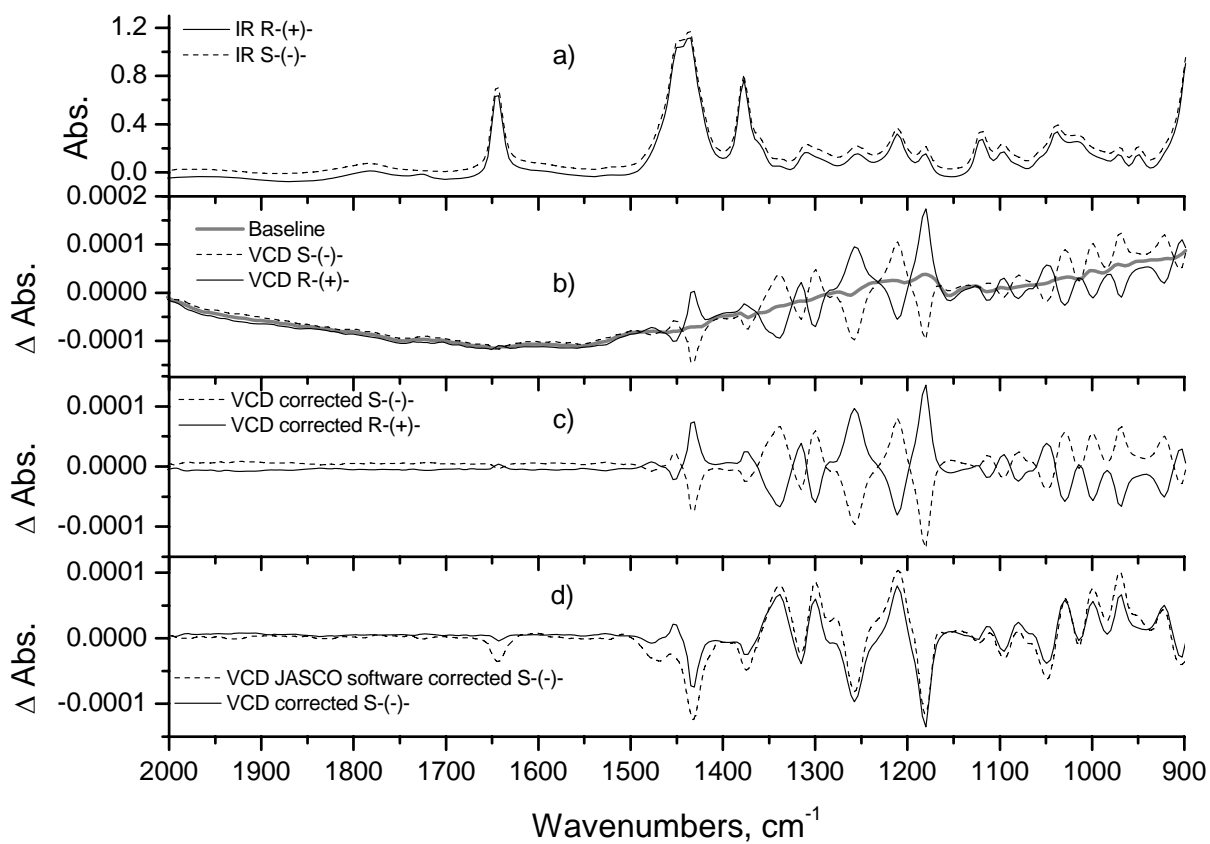
Dr. Juan Jesús López González.

Grupo de Química Física Teórica y Experimental FQM173, Edificio B3. Campus las Lagunillas, Facultad de Ciencias Experimentales, Universidad de Jaén, E-23071 Jaén, Spain.

Tel : +34-953 21 27 54; Fax : +34-953-21 29 40

E-mail : [jjlopez@ujaen.es](mailto:jjlopez@ujaen.es)

**Figure 1S.** Experimental IR and VCD spectra of S-(-)-limonene oxide and R-(+)-limonene oxide in the 2000  $\text{cm}^{-1}$ - 900  $\text{cm}^{-1}$  spectral region: a) IR spectra (16  $\text{cm}^{-1}$  resolution); b) raw VCD spectra and baseline obtained as the half-sum of the VCD spectra of enantiomers (neat liquid, 4000 scans, 8  $\text{cm}^{-1}$  of resolution, spacer of 15  $\mu\text{m}$ ); c) baseline corrected VCD spectra; d) comparison between corrected S-enantiomer spectra obtained as indicated above and as corrected using JASCO software (figure 6 of the manuscript).



**Table 1S:** Calculated equilibrium structures of S-(-)-Limonene oxide at B3LYP/ cc-pVDZ levels for the six equatorial conformers (eq-t110, eq-t255, eq-t305, eq-c110, eq-c255, eq-c305) and the six axial conformers (ax-t115, ax-t240, ax-t345, ax-c115, ax-c240, ax-c345). Atoms are numerated in *figure 1*.

The following *Z*-matrix in internal coordinates has been used:

C							
C	1	B1					
C	2	B2	1	A1			
C	3	B3	2	A2	1	D1	0
C	4	B4	3	A3	2	D2	0
C	1	B5	2	A4	3	D3	0
C	4	B6	3	A5	2	D4	0
C	7	B7	4	A6	3	D5	0
C	7	B8	4	A7	8	D6	1
C	1	B9	2	A8	3	D7	0
H	8	B10	7	A9	9	D8	0
H	8	B11	7	A10	9	D9	0
H	9	B12	7	A11	8	D10	0
H	9	B13	7	A12	8	D11	0
H	9	B14	7	A13	8	D12	0
H	2	B15	1	A14	10	D13	0
H	3	B16	2	A15	1	D14	0
H	3	B17	2	A16	1	D15	0
H	4	B18	3	A17	2	D16	0
H	5	B19	4	A18	3	D17	0
H	5	B20	4	A19	3	D18	0
H	6	B21	1	A20	2	D19	0
H	6	B22	1	A21	2	D20	0
H	10	B23	1	A22	2	D21	0
H	10	B24	1	A23	2	D22	0
H	10	B25	1	A24	2	D23	0
O	1	B26	2	A25	3	D24	0

Bond length: B1-B26 in Ångstroms.

Angles: A1-A25 in degrees.

Dihedral angles: D1-D24 in degrees.

Supplementary Material (ESI) for PCCP

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Supplementary Material (ESI) for *PCCP*  
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D2=50.47870372 D3=1.91032255 D4=79.17021481 D5=154.64263598 D6=120.04861808 D7=154.81236909 D8=0.09239126 D9=179.98459394 D10=5.50333168 D11=126.1009836 D12=114.43374857 D13=2.0415138 D14=147.39416113 D15=98.09331895 D16=165.05362588 D17=172.52166167 D18=57.23388175 D19=109.93146174 D20=134.83317065 D21=27.45320459 D22=93.60283693 D23=147.02730618 D24=100.97303543	B1=1.4807387 B2=1.51506624 B3=1.55067245 B4=1.54848721 B5=1.52804762 B6=1.52784715 B7=1.34020515 B8=1.51143413 B9=1.51169046 B10=1.09399865 B11=1.09001999 B12=1.09992538 B13=1.10447816 B14=1.10523733 B15=1.09981799 B16=1.10280812 B17=1.10514062 B18=1.10464079 B19=1.10207791 B20=1.10567693 B21=1.10209357 B22=1.10233374 B23=1.09995482 B24=1.10283165 B25=1.10328518 B26=1.43708338 A1=122.5337778 A2=116.61006407 A3=109.59630869 A4=118.38778066 A5=116.83033854 A6=124.46659762 A7=114.33648332 A8=120.39546026 A9=120.42487192 A10=121.92206387 A11=111.74598815 A12=111.61128989 A13=110.96672386 A14=117.62269071 A15=109.40392894 A16=105.90060225 A17=105.78356497 A18=110.25262379 A19=108.04929583 A20=108.04515969 A21=109.41805119 A22=110.88434272 A23=110.96091761 A24=110.28787173 A25=59.57285505 D1=10.19467238 D2=36.26624779 D3=3.31612776 D4=93.10989321 D5=29.17066979 D6=121.19598467 D7=152.53462691 D8=0.07525961 D9=178.17515928 D10=3.51100093 D11=124.3805191 D12=117.31374124 D13=0.89056996 D14=136.33988202 D15=109.70698868 D16=150.23013504 D17=178.03531853 D18=62.36015098 D19=98.29631968 D20=145.73485999 D21=26.52021414 D22=94.5101541 D23=146.2110898 D24=101.05185713	B1=1.4826227 B2=1.52089352 B3=1.54778154 B4=1.54897117 B5=1.51975647 B6=1.53093756 B7=1.34134955 B8=1.51186366 B9=1.51217053 B10=1.09342724 B11=1.09394395 B12=1.10003229 B13=1.10350893 B14=1.10162214 B15=1.09886174 B16=1.10193997 B17=1.10316439 B18=1.10755047 B19=1.10110191 B20=1.10285722 B21=1.1034316 B22=1.10469209 B23=1.09981626 B24=1.10309913 B25=1.10267034 B26=1.44318015 A1=123.09737968 A2=114.75645894 A3=109.8046758 A4=118.99326209 A5=113.9998591 A6=119.61790249 A7=120.05613436 A8=120.34917323 A9=121.60437957 A10=121.52930766 A11=110.87369043 A12=111.49175004 A13=112.44136921 A14=117.22344815 A15=109.66499167 A16=106.6293955 A17=107.17453263 A18=109.45323075 A19=107.82376539 A20=108.82048824 A21=108.39438857 A22=110.79058392 A23=110.28203053 A24=111.20939137 A25=59.05454779 D1=11.25089587 D2=39.18104682 D3=0.44843241 D4=89.28679541 D5=141.59032728 D6=120.3209294 D7=155.79491224 D8=1.79535583 D9=178.8532667 D10=0.03283424 D11=119.8420856 D12=120.9219204 D13=0.37535944 D14=136.18672267 D15=109.3435148 D16=154.12896797 D17=176.67311415 D18=60.25209013 D19=104.14377557 D20=141.03408373 D21=26.81263441 D22=146.35522353 D23=94.22983841 D24=102.17282289	B1=1.48004525 B2=1.51984616 B3=1.55255727 B4=1.54067078 B5=1.51778459 B6=1.53131282 B7=1.34131898 B8=1.51289631 B9=1.512105 B10=1.0932907 B11=1.09042538 B12=1.09966393 B13=1.10443165 B14=1.10346273 B15=1.09873287 B16=1.09947027 B17=1.10305789 B18=1.10750547 B19=1.10114541 B20=1.10196435 B21=1.10166956 B22=1.10469112 B23=1.09985388 B24=1.1031595 B25=1.10251155 B26=1.44409599 A1=122.8241273 A2=114.71205784 A3=109.0279630 A4=118.87525006 A5=114.33154257 A6=123.75929305 A7=116.4240494 A8=120.36264914 A9=120.70402113 A10=123.00046985 A11=111.08684967 A12=111.32650325 A13=112.05237143 A14=117.38289692 A15=109.30926091 A16=106.65373089 A17=105.6962269 A18=110.63737112 A19=107.71623005 A20=107.83132417 A21=108.48238814 A22=110.7579453 A23=110.33907657 A24=111.0543206 A25=59.11826876 D1=13.12118372 D2=41.57370875 D3=0.69863608 D4=89.47522959 D5=139.57493032 D6=119.63105746 D7=155.49898313 D8=0.29041677 D9=178.85326677 D10=9.02980357 D11=129.57099117 D12=111.23530042 D13=0.54761206 D14=138.53398504 D15=107.24079427 D16=156.52952520 D17=174.58482091 D18=58.59011441 D19=104.58770086 D20=140.38436301 D21=27.42665209 D22=146.96853349 D23=93.56108704 D24=102.28650308	B1=1.48044285 B2=1.52074848 B3=1.54329731 B4=1.55073935 B5=1.51950227 B6=1.52587834 B7=1.34092913 B8=1.5107602 B9=1.51159114 B10=1.09329473 B11=1.09161177 B12=1.0997808 B13=1.10365187 B14=1.10462488 B15=1.09889405 B16=1.10117648 B17=1.10323649 B18=1.10524333 B19=1.10107787 B20=1.10182942 B21=1.10358353 B22=1.10447875 B23=1.09987429 B24=1.10313715 B25=1.10252847 B26=1.4437967 A1=122.76302451 A2=114.69457591 A3=109.30438478 A4=118.72413758 A5=115.03007311 A6=124.04756094 A7=115.23079375 A8=120.45330812 A9=120.94684718 A10=122.60171073 A11=111.66755321 A12=111.70760612 A13=110.82897245 A14=117.3968637 A15=109.64915754 A16=106.74943324 A17=107.32765243 A18=110.69870443 A19=108.2522776 A20=108.25700134 A21=108.67205066 A22=110.8025748 A23=110.36520658 A24=110.98603147 A25=59.15451122 D1=10.70548228 D2=40.45625198 D3=0.08420315 D4=86.21413923 D5=16.83231456 D6=120.72085169 D7=154.95519062 D8=0.2915289 D9=179.79175009 D10=0.8106342 D11=120.05712736 D12=121.54075058 D13=0.64696875 D14=135.23551532 D15=109.85671207 D16=156.04191611 D17=174.19394281 D18=57.34821222 D19=101.40033445 D20=143.06229420 D21=27.02404348 D22=146.62077888 D23=93.94153541 D24=102.3557283

**Table 2S:** Theoretical (B3LYP/ cc-pVDZ) vibrational wavenumbers, infrared intensities, Raman activities, dipole strengths and rotatory strengths for the five most stable equatorial conformers (eq-t110, eq-t255, eq-c110, eq-c255 and eq-c305) of the S(-)-Limonene oxide.

S(-)-Limonene Oxide, eq-t110 (0.0 kJ/mol)

Harmonic frequencies (cm<sup>-1</sup>), IR intensities (KM/Mole), Raman scattering activities (A<sup>4</sup>/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), Dipole strengths (10<sup>-40</sup> esu<sup>2</sup>-cm<sup>2</sup>), Rotational strengths (10<sup>-44</sup> esu<sup>2</sup>-cm<sup>2</sup>), and normal coordinates:

	75	74	73
	A	A	A
Frequencies --	54.3744	65.4390	165.8162
Red. masses --	2.6383	3.2395	2.4730
Frc consts --	0.0046	0.0082	0.0401
IR Inten --	0.5811	0.9157	0.2689
Raman Activ --	5.0382	0.8132	1.0925
Depolar (P) --	0.7492	0.7422	0.7365
Depolar (U) --	0.8566	0.8520	0.8482
Dip. str. --	42.6372	55.8263	6.4699
Rot. str. --	-2.2953	1.8552	0.4776
	72	71	70
	A	A	A
Frequencies --	178.2733	187.7392	209.0620
Red. masses --	1.2561	1.1285	2.2788
Frc consts --	0.0235	0.0234	0.0587
IR Inten --	0.1582	0.3627	0.8156
Raman Activ --	0.6160	0.2180	0.4918
Depolar (P) --	0.7145	0.7007	0.6630
Depolar (U) --	0.8335	0.8240	0.7973
Dip. str. --	3.5397	7.7074	15.5645
Rot. str. --	2.7371	1.5352	1.9889
	69	68	67
	A	A	A
Frequencies --	234.2876	282.5798	318.1149
Red. masses --	2.0940	3.3990	2.2314
Frc consts --	0.0677	0.1599	0.1330
IR Inten --	0.9219	0.8213	1.2690
Raman Activ --	0.3294	2.1144	1.7673
Depolar (P) --	0.2465	0.3068	0.6582
Depolar (U) --	0.3955	0.4696	0.7938
Dip. str. --	15.6979	11.5944	15.9147
Rot. str. --	-3.5104	-0.8807	1.9369
	66	65	64
	A	A	A
Frequencies --	318.5961	389.3903	442.1619
Red. masses --	2.5866	2.3743	2.5550
Frc consts --	0.1547	0.2121	0.2943
IR Inten --	0.3795	5.1335	5.9600
Raman Activ --	1.4771	0.9412	0.7367
Depolar (P) --	0.6335	0.6085	0.3411
Depolar (U) --	0.7756	0.7566	0.5086
Dip. str. --	4.7523	52.5943	53.7737
Rot. str. --	-0.1644	-3.7267	-7.6245
	63	62	61
	A	A	A
Frequencies --	471.2945	508.4202	533.3810
Red. masses --	2.5668	2.9481	2.7419
Frc consts --	0.3359	0.4490	0.4596
IR Inten --	0.1488	5.4902	2.5347
Raman Activ --	0.7232	3.6121	3.1463
Depolar (P) --	0.7443	0.1015	0.6011
Depolar (U) --	0.8534	0.1843	0.7509
Dip. str. --	1.2597	43.0800	18.9585
Rot. str. --	1.2430	-3.7252	0.2372
	60	59	58
	A	A	A
Frequencies --	564.5928	615.8598	686.2351
Red. masses --	2.8914	2.9734	3.8756
Frc consts --	0.5430	0.6644	1.0753
IR Inten --	7.2119	0.3977	5.1902
Raman Activ --	1.3593	1.6266	9.6501
Depolar (P) --	0.6804	0.7439	0.1589
Depolar (U) --	0.8098	0.8531	0.2743
Dip. str. --	50.9594	2.5760	30.1729
Rot. str. --	-3.4835	6.6101	-13.0300
	57	56	55
	A	A	A
Frequencies --	727.1400	765.8340	808.4666
Red. masses --	1.1557	2.9397	2.1342
Frc consts --	0.3600	1.0158	0.8219
IR Inten --	0.7139	8.1689	4.4569
Raman Activ --	3.5564	14.2322	2.5887
Depolar (P) --	0.4741	0.1880	0.5988
Depolar (U) --	0.6433	0.3165	0.7490
Dip. str. --	3.9168	42.5536	21.9925
Rot. str. --	10.9213	4.9539	7.9921
	54	53	52
	A	A	A
Frequencies --	860.4676	896.9499	901.5241

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Red. masses	--	2.7584	2.1500	2.1030
Frc consts	--	1.2033	1.0191	1.0070
IR Inten	--	12.0478	4.7361	3.3329
Raman Activ	--	1.8923	5.6200	1.5435
Depolar (P)	--	0.4352	0.3397	0.6980
Depolar (U)	--	0.6064	0.5071	0.8221
Dip. str.	--	55.8573	21.0650	14.7488
Rot. str.	--	-2.7220	-3.6065	0.9582
		51	50	49
		A	A	A
Frequencies	--	919.1968	926.5789	986.2541
Red. masses	--	1.3699	1.8070	1.9813
Frc consts	--	0.6820	0.9141	1.1355
IR Inten	--	33.4138	0.8801	2.2232
Raman Activ	--	0.2265	0.7636	1.0585
Depolar (P)	--	0.7031	0.1319	0.6330
Depolar (U)	--	0.8257	0.2330	0.7752
Dip. str.	--	145.0187	3.7895	8.9929
Rot. str.	--	-25.6171	3.0304	-4.9551
		48	47	46
		A	A	A
Frequencies	--	990.5512	1009.3446	1025.9948
Red. masses	--	1.4036	1.4257	2.0894
Frc consts	--	0.8114	0.8557	1.2959
IR Inten	--	1.5963	5.1067	6.4968
Raman Activ	--	0.6601	2.8910	4.4205
Depolar (P)	--	0.7117	0.7500	0.1988
Depolar (U)	--	0.8315	0.8571	0.3316
Dip. str.	--	6.4290	20.1840	25.2615
Rot. str.	--	17.3037	-23.0592	3.5764
		45	44	43
		A	A	A
Frequencies	--	1041.8106	1051.0444	1056.6449
Red. masses	--	1.5765	1.5041	1.5589
Frc consts	--	1.0081	0.9790	1.0255
IR Inten	--	3.0544	2.9023	1.0782
Raman Activ	--	5.0536	6.7965	0.9870
Depolar (P)	--	0.7492	0.7459	0.7324
Depolar (U)	--	0.8566	0.8545	0.8455
Dip. str.	--	11.6963	11.0162	4.0706
Rot. str.	--	-10.9055	-16.4863	13.8265
		42	41	40
		A	A	A
Frequencies	--	1096.9966	1104.6818	1132.9765
Red. masses	--	2.1548	2.1731	2.6057
Frc consts	--	1.5278	1.5625	1.9707
IR Inten	--	3.5810	7.9672	8.8199
Raman Activ	--	2.8301	4.8760	2.4725
Depolar (P)	--	0.2318	0.6748	0.6894
Depolar (U)	--	0.3763	0.8059	0.8161
Dip. str.	--	13.0230	28.7725	31.0564
Rot. str.	--	-6.0771	-6.4038	-10.6400
		39	38	37
		A	A	A
Frequencies	--	1201.1126	1223.2484	1231.5315
Red. masses	--	1.4455	1.6339	1.4382
Frc consts	--	1.2286	1.4404	1.2852
IR Inten	--	1.2189	13.0137	3.2397
Raman Activ	--	1.7032	7.8608	2.3377
Depolar (P)	--	0.5836	0.6923	0.7280
Depolar (U)	--	0.7371	0.8182	0.8426
Dip. str.	--	4.0483	42.4417	10.4947
Rot. str.	--	13.0281	1.8370	-9.8762
		36	35	34
		A	A	A
Frequencies	--	1271.8708	1298.2323	1307.5949
Red. masses	--	1.3976	2.8043	1.2205
Frc consts	--	1.3321	2.7847	1.2296
IR Inten	--	3.6988	3.7707	1.1157
Raman Activ	--	3.7495	0.6473	9.9301
Depolar (P)	--	0.5892	0.4520	0.5503
Depolar (U)	--	0.7415	0.6225	0.7099
Dip. str.	--	11.6019	11.5873	3.4038
Rot. str.	--	15.0646	1.4815	3.0897
		33	32	31
		A	A	A
Frequencies	--	1321.0146	1328.5996	1364.1964
Red. masses	--	1.2604	1.3959	1.4014
Frc consts	--	1.2959	1.4518	1.5366
IR Inten	--	2.7712	4.4606	2.2609
Raman Activ	--	8.0520	3.8670	4.8032
Depolar (P)	--	0.5927	0.5448	0.6892
Depolar (U)	--	0.7442	0.7054	0.8160
Dip. str.	--	8.3690	13.3940	6.6118
Rot. str.	--	-7.9872	23.6981	-9.6315
		30	29	28
		A	A	A
Frequencies	--	1379.0330	1383.8811	1396.4718
Red. masses	--	1.5878	1.5988	1.3607
Frc consts	--	1.7791	1.8040	1.5634
IR Inten	--	0.7700	1.8435	0.9875
Raman Activ	--	5.4724	3.4006	3.6156
Depolar (P)	--	0.4091	0.7398	0.6059
Depolar (U)	--	0.5806	0.8504	0.7546
Dip. str.	--	2.2275	5.3143	2.8212
Rot. str.	--	-2.7454	6.0277	7.4887
		27	26	25
		A	A	A
Frequencies	--	1398.3006	1430.1713	1442.8460
Red. masses	--	1.3753	1.1741	1.2534
Frc consts	--	1.5843	1.4149	1.5374
IR Inten	--	13.1765	0.1672	3.0659
Raman Activ	--	3.6147	22.1754	28.4106
Depolar (P)	--	0.7424	0.4831	0.7129
Depolar (U)	--	0.8522	0.6515	0.8324
Dip. str.	--	37.5929	0.4663	8.4771
Rot. str.	--	-9.7676	-0.4315	0.1819

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	24	23	22
	A	A	A
Frequencies --	1446.4991	1448.4297	1452.0763
Red. masses --	1.1150	1.0824	1.0623
Frc consts --	1.3746	1.3379	1.3197
IR Inten --	4.7712	3.4740	9.2243
Raman Activ --	6.3794	3.1964	14.9657
Depolar (P) --	0.5731	0.7201	0.7478
Depolar (U) --	0.7287	0.8373	0.8557
Dip. str. --	13.1589	9.5683	25.3425
Rot. str. --	15.6105	1.9653	0.8608
	21	20	19
	A	A	A
Frequencies --	1460.7771	1466.6541	1467.7823
Red. masses --	1.0749	1.0716	1.0943
Frc consts --	1.3514	1.3581	1.3890
IR Inten --	8.1706	11.4713	2.2843
Raman Activ --	12.2399	6.5424	4.3075
Depolar (P) --	0.7492	0.7226	0.6764
Depolar (U) --	0.8566	0.8390	0.8070
Dip. str. --	22.3140	31.2027	6.2087
Rot. str. --	-5.3058	-5.8881	-2.5107
	18	17	16
	A	A	A
Frequencies --	1495.1839	1714.7129	3006.8369
Red. masses --	2.3504	5.5544	1.0809
Frc consts --	3.0958	9.6221	5.7578
IR Inten --	6.9984	19.0776	9.9637
Raman Activ --	4.5506	29.3685	38.1458
Depolar (P) --	0.2555	0.1725	0.5577
Depolar (U) --	0.4070	0.2943	0.7161
Dip. str. --	18.6730	44.3852	13.2196
Rot. str. --	13.6975	-1.7668	-14.5978
	15	14	13
	A	A	A
Frequencies --	3011.0170	3024.0964	3028.2543
Red. masses --	1.0619	1.0399	1.0379
Frc consts --	5.6723	5.6030	5.6076
IR Inten --	34.1740	12.3078	37.6973
Raman Activ --	87.6012	428.6812	164.4477
Depolar (P) --	0.1662	0.4952	0.0289
Depolar (U) --	0.2850	0.6624	0.0561
Dip. str. --	45.2783	16.2365	49.6622
Rot. str. --	10.6488	-20.2313	-12.6741
	12	11	10
	A	A	A
Frequencies --	3031.7345	3039.2070	3050.3130
Red. masses --	1.0594	1.0684	1.0938
Frc consts --	5.7370	5.8144	5.9963
IR Inten --	25.7213	15.6948	36.3495
Raman Activ --	126.2502	122.9988	115.6233
Depolar (P) --	0.2143	0.1052	0.2835
Depolar (U) --	0.3530	0.1904	0.4418
Dip. str. --	33.8462	20.6016	47.5403
Rot. str. --	22.8392	-33.6312	28.4563
	9	8	7
	A	A	A
Frequencies --	3072.0900	3078.7209	3087.5272
Red. masses --	1.1006	1.0986	1.0966
Frc consts --	6.1198	6.1353	6.1590
IR Inten --	11.9208	28.0974	36.9866
Raman Activ --	64.2126	747.1282	116.7125
Depolar (P) --	0.6242	0.7484	0.3510
Depolar (U) --	0.7686	0.8561	0.5196
Dip. str. --	15.4802	36.4086	47.7904
Rot. str. --	30.2078	-22.0208	-21.7268
	6	5	4
	A	A	A
Frequencies --	3089.9491	3094.5557	3116.6009
Red. masses --	1.0979	1.1009	1.1007
Frc consts --	6.1762	6.2112	6.2993
IR Inten --	29.6291	29.1079	22.8152
Raman Activ --	110.0853	85.6032	161.4995
Depolar (P) --	0.3892	0.7493	0.7398
Depolar (U) --	0.5603	0.8567	0.8505
Dip. str. --	38.2538	37.5250	29.2045
Rot. str. --	11.0439	-16.4406	0.6243
	3	2	1
	A	A	A
Frequencies --	3121.8161	3128.9718	3218.4550
Red. masses --	1.1016	1.0608	1.1156
Frc consts --	6.3253	6.1189	6.8087
IR Inten --	19.9521	10.6078	20.2924
Raman Activ --	77.6553	144.9458	91.6262
Depolar (P) --	0.6860	0.1356	0.7165
Depolar (U) --	0.8137	0.2389	0.8348
Dip. str. --	25.4969	13.5248	25.1532
Rot. str. --	3.5524	10.6925	15.3623

## S-(-)-Limonene Oxide, eq-t255 (1.9 kJ/mol)

Harmonic frequencies (cm<sup>-1</sup>), IR intensities (KM/Mole), Raman scattering activities (A<sup>4</sup>/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), Dipole strengths (10<sup>-40</sup> esu<sup>2</sup>-cm<sup>2</sup>), Rotational strengths (10<sup>-44</sup> esu<sup>2</sup>-cm<sup>2</sup>), and normal coordinates:

	75	74	73
	A	A	A
Frequencies --	43.2349	67.7663	172.3330
Red. masses --	2.6335	3.2331	2.0986
Frc consts --	0.0029	0.0087	0.0367
IR Inten --	0.1164	0.5806	0.4133
Raman Activ --	2.8535	0.3776	1.0535



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Depolar (P) --	0.7491	0.7500	0.7257
Depolar (U) --	0.8565	0.8571	0.8411
Dip. str. --	10.7427	34.1806	9.5674
Rot. str. --	-1.0686	-1.2162	0.2353
	72	71	70
	A	A	A
Frequencies --	179.9088	186.8771	209.7194
Red. masses --	1.1336	1.3471	2.1758
Frc consts --	0.0216	0.0277	0.0564
IR Inten --	0.5071	0.1573	1.0958
Raman Activ --	0.0572	0.5246	0.6466
Depolar (P) --	0.7160	0.7346	0.7219
Depolar (U) --	0.8345	0.8470	0.8385
Dip. str. --	11.2454	3.3586	20.8454
Rot. str. --	-0.7357	2.7835	-2.3957
	69	68	67
	A	A	A
Frequencies --	241.7411	286.3539	317.9392
Red. masses --	2.1874	3.7222	2.5399
Frc consts --	0.0753	0.1798	0.1513
IR Inten --	0.9155	0.1381	1.7687
Raman Activ --	0.7553	2.5696	0.4315
Depolar (P) --	0.4390	0.3047	0.2960
Depolar (U) --	0.6102	0.4670	0.4567
Dip. str. --	15.1088	1.9240	22.1932
Rot. str. --	4.4809	0.6603	6.4317
	66	65	64
	A	A	A
Frequencies --	334.9659	392.9259	430.6567
Red. masses --	2.2532	2.3090	2.9737
Frc consts --	0.1490	0.2100	0.3249
IR Inten --	0.6325	5.1978	3.0186
Raman Activ --	1.8172	1.0398	0.6823
Depolar (P) --	0.7464	0.3584	0.6786
Depolar (U) --	0.8548	0.5277	0.8085
Dip. str. --	7.5331	52.7734	27.9632
Rot. str. --	0.7353	-2.8558	-7.2398
	63	62	61
	A	A	A
Frequencies --	459.3628	492.6721	546.0809
Red. masses --	2.7012	2.7057	2.5030
Frc consts --	0.3358	0.3869	0.4398
IR Inten --	3.9983	1.4332	1.4712
Raman Activ --	0.8588	1.6690	4.0201
Depolar (P) --	0.7482	0.4092	0.2848
Depolar (U) --	0.8559	0.5808	0.4433
Dip. str. --	34.7240	11.6054	10.7481
Rot. str. --	-5.0280	-10.7225	-9.0541
	60	59	58
	A	A	A
Frequencies --	558.0639	616.2449	688.2148
Red. masses --	3.0166	2.9532	3.9432
Frc consts --	0.5535	0.6608	1.1004
IR Inten --	7.3995	0.5140	5.5869
Raman Activ --	1.6836	1.5584	11.1238
Depolar (P) --	0.6949	0.7308	0.1605
Depolar (U) --	0.8200	0.8445	0.2767
Dip. str. --	52.8961	3.3278	32.3856
Rot. str. --	25.5490	7.5581	-5.4163
	57	56	55
	A	A	A
Frequencies --	713.9844	774.9242	818.9456
Red. masses --	1.2053	2.7104	1.8849
Frc consts --	0.3620	0.9590	0.7448
IR Inten --	0.4987	7.1172	5.3156
Raman Activ --	6.3689	12.1035	0.8192
Depolar (P) --	0.3657	0.2946	0.3201
Depolar (U) --	0.5356	0.4551	0.4849
Dip. str. --	2.7864	36.6400	25.8943
Rot. str. --	2.0531	5.7809	6.2318
	54	53	52
	A	A	A
Frequencies --	863.7317	899.8402	913.3714
Red. masses --	2.9090	1.8972	2.2464
Frc consts --	1.2786	0.9051	1.1042
IR Inten --	13.9804	2.7590	3.8965
Raman Activ --	2.8283	2.1278	4.6195
Depolar (P) --	0.4979	0.7272	0.3877
Depolar (U) --	0.6648	0.8421	0.5588
Dip. str. --	64.5728	12.2317	17.0191
Rot. str. --	2.8033	-11.5625	16.4830
	51	50	49
	A	A	A
Frequencies --	921.1603	927.1475	983.0285
Red. masses --	1.4217	1.8924	1.8640
Frc consts --	0.7108	0.9584	1.0613
IR Inten --	29.9674	2.2436	2.8706
Raman Activ --	0.6588	1.6450	1.4340
Depolar (P) --	0.4140	0.1094	0.7346
Depolar (U) --	0.5856	0.1972	0.8470
Dip. str. --	129.7839	9.6541	11.6498
Rot. str. --	-10.4612	-0.0385	-9.9135
	48	47	46
	A	A	A
Frequencies --	997.2853	1003.1976	1019.8663
Red. masses --	1.6683	1.4181	1.8073
Frc consts --	0.9776	0.8409	1.1075
IR Inten --	1.5017	4.3935	4.4355
Raman Activ --	1.5946	4.4870	0.6790
Depolar (P) --	0.4286	0.7040	0.6894
Depolar (U) --	0.6000	0.8263	0.8162
Dip. str. --	6.0071	17.4717	17.3503
Rot. str. --	-1.2388	-15.0126	33.5212
	45	44	43
	A	A	A
Frequencies --	1039.2986	1052.1529	1056.0378
Red. masses --	1.7080	1.4467	1.5611

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Frc consts	--	1.0870	0.9436	1.0258
IR Inten	--	4.2748	0.8610	2.8216
Raman Activ	--	3.4499	6.5502	2.2619
Depolar (P)	--	0.3150	0.7385	0.7498
Depolar (U)	--	0.4791	0.8496	0.8570
Dip. str.	--	16.4090	3.2645	10.6593
Rot. str.	--	-23.2088	-6.9504	7.3501
		42	41	40
		A	A	A
Frequencies	--	1098.9442	1110.4626	1139.2178
Red. masses	--	2.1117	2.2190	2.5475
Frc consts	--	1.5026	1.6122	1.9480
IR Inten	--	0.9565	11.1631	4.2359
Raman Activ	--	2.9063	3.1593	2.2065
Depolar (P)	--	0.1082	0.6821	0.7498
Depolar (U)	--	0.1952	0.8110	0.8570
Dip. str.	--	3.4723	40.1042	14.8337
Rot. str.	--	1.5436	10.3177	-8.6360
		39	38	37
		A	A	A
Frequencies	--	1199.9862	1219.9034	1225.5819
Red. masses	--	1.4374	1.3502	1.7899
Frc consts	--	1.2195	1.1838	1.5841
IR Inten	--	1.1916	5.4541	17.0413
Raman Activ	--	1.3908	6.7353	4.4487
Depolar (P)	--	0.6032	0.6424	0.7068
Depolar (U)	--	0.7525	0.7823	0.8282
Dip. str.	--	3.9616	17.8364	55.4712
Rot. str.	--	13.1185	-18.0466	-13.5077
		36	35	34
		A	A	A
Frequencies	--	1263.9822	1276.8407	1316.9175
Red. masses	--	1.5880	1.4967	1.3458
Frc consts	--	1.4948	1.4376	1.3752
IR Inten	--	2.4962	4.5343	1.0909
Raman Activ	--	2.6393	2.5371	9.7718
Depolar (P)	--	0.4758	0.7396	0.7483
Depolar (U)	--	0.6448	0.8503	0.8560
Dip. str.	--	7.8785	14.1672	3.3049
Rot. str.	--	6.0540	13.1883	18.6134
		33	32	31
		A	A	A
Frequencies	--	1322.7217	1337.7138	1354.5261
Red. masses	--	1.3053	1.4540	1.4498
Frc consts	--	1.3456	1.5330	1.5673
IR Inten	--	5.6619	1.7548	1.6980
Raman Activ	--	7.1525	1.1995	5.5722
Depolar (P)	--	0.5228	0.7133	0.5708
Depolar (U)	--	0.6866	0.8327	0.7267
Dip. str.	--	17.0766	5.2331	5.0009
Rot. str.	--	-5.9334	14.7852	-2.9811
		30	29	28
		A	A	A
Frequencies	--	1381.7732	1393.3824	1397.2876
Red. masses	--	1.7574	1.2664	1.3893
Frc consts	--	1.9770	1.4486	1.5982
IR Inten	--	1.5232	3.6358	7.7769
Raman Activ	--	2.5150	5.1916	2.7889
Depolar (P)	--	0.2070	0.6445	0.6761
Depolar (U)	--	0.3430	0.7838	0.8068
Dip. str.	--	4.3978	10.4097	22.2037
Rot. str.	--	0.5283	-4.0164	3.1218
		27	26	25
		A	A	A
Frequencies	--	1402.0446	1428.9510	1443.6690
Red. masses	--	1.7054	1.1709	1.2819
Frc consts	--	1.9751	1.4086	1.5741
IR Inten	--	0.8569	0.5833	3.3828
Raman Activ	--	4.7485	32.2556	26.1768
Depolar (P)	--	0.7189	0.5693	0.6663
Depolar (U)	--	0.8365	0.7256	0.7997
Dip. str.	--	2.4382	1.6286	9.3479
Rot. str.	--	-0.2457	-1.2201	-5.9957
		24	23	22
		A	A	A
Frequencies	--	1447.6619	1450.1593	1452.3257
Red. masses	--	1.0904	1.0869	1.0543
Frc consts	--	1.3464	1.3467	1.3102
IR Inten	--	7.2699	6.3274	2.9432
Raman Activ	--	4.4210	1.8320	7.5554
Depolar (P)	--	0.7104	0.5986	0.7490
Depolar (U)	--	0.8307	0.7489	0.8565
Dip. str.	--	20.0340	17.4068	8.0846
Rot. str.	--	4.3915	3.8288	-0.5944
		21	20	19
		A	A	A
Frequencies	--	1460.8801	1465.7247	1470.1093
Red. masses	--	1.0736	1.0729	1.0979
Frc consts	--	1.3500	1.3580	1.3980
IR Inten	--	7.1234	15.8748	0.1606
Raman Activ	--	13.3301	4.5789	4.5908
Depolar (P)	--	0.7495	0.7011	0.6951
Depolar (U)	--	0.8568	0.8243	0.8201
Dip. str.	--	19.4528	43.2079	0.4359
Rot. str.	--	6.7849	-4.7486	1.6397
		18	17	16
		A	A	A
Frequencies	--	1496.2724	1716.6744	2967.3942
Red. masses	--	2.3709	5.4827	1.0813
Frc consts	--	3.1274	9.5196	5.6098
IR Inten	--	5.4261	19.6312	22.9713
Raman Activ	--	4.1979	22.8321	62.4501
Depolar (P)	--	0.2571	0.1265	0.2704
Depolar (U)	--	0.4090	0.2246	0.4256
Dip. str.	--	14.4671	45.6212	30.8828
Rot. str.	--	12.5387	5.8295	-12.6224
		15	14	13

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A			
Frequencies --	3010.3486	3015.4286	3027.3906
Red. masses --	1.0599	1.0396	1.0605
Frc consts --	5.6590	5.5697	5.7266
IR Inten --	29.3399	23.8582	33.1855
Raman Activ --	52.2591	143.3552	44.6887
Depolar (P) --	0.2040	0.0182	0.2161
Depolar (U) --	0.3388	0.0358	0.3554
Dip. str. --	38.8820	31.5643	43.7308
Rot. str. --	-4.4582	14.3865	-1.2463
12			
A			
Frequencies --	3028.2750	3041.1950	3052.6385
Red. masses --	1.0388	1.0755	1.0853
Frc consts --	5.6126	5.8607	5.9585
IR Inten --	26.5229	11.0953	34.7961
Raman Activ --	219.1263	72.8882	100.2980
Depolar (P) --	0.0281	0.3769	0.1920
Depolar (U) --	0.0547	0.5474	0.3221
Dip. str. --	34.9408	14.5547	45.4739
Rot. str. --	24.5218	-24.7294	35.1566
9			
A			
Frequencies --	3066.6612	3073.4995	3088.0249
Red. masses --	1.0994	1.0983	1.0925
Frc consts --	6.0918	6.1127	6.1383
IR Inten --	26.9037	8.7273	58.9848
Raman Activ --	61.5238	48.0734	125.3312
Depolar (P) --	0.7161	0.7109	0.2019
Depolar (U) --	0.8346	0.8310	0.3360
Dip. str. --	34.9989	11.3281	76.2021
Rot. str. --	-21.2501	21.3687	-30.9413
6			
A			
Frequencies --	3091.8403	3094.4799	3114.8821
Red. masses --	1.1035	1.1010	1.1001
Frc consts --	6.2150	6.2116	6.2886
IR Inten --	13.3494	30.8793	23.3521
Raman Activ --	91.9207	80.8164	77.0964
Depolar (P) --	0.4511	0.7373	0.6798
Depolar (U) --	0.6217	0.8488	0.8093
Dip. str. --	17.2248	39.8095	29.9083
Rot. str. --	9.2689	-2.1302	-6.7541
3			
A			
Frequencies --	3121.7011	3143.2220	3234.0211
Red. masses --	1.1016	1.0618	1.1139
Frc consts --	6.3247	6.1810	6.8639
IR Inten --	20.1483	9.2146	16.2011
Raman Activ --	77.1837	149.2426	66.2113
Depolar (P) --	0.6877	0.1568	0.7496
Depolar (U) --	0.8149	0.2711	0.8569
Dip. str. --	25.7487	11.6953	19.9852
Rot. str. --	-6.0091	1.1135	3.9589

S-(-)-Limonene Oxide, eq-c110 (2.0 kJ/mol)

Harmonic frequencies (cm<sup>-1</sup>), IR intensities (KM/Mole), Raman scattering activities (A<sup>4</sup>/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), Dipole strengths (10<sup>-40</sup> esu<sup>2</sup>-cm<sup>2</sup>), Rotational strengths (10<sup>-44</sup> esu<sup>2</sup>-cm<sup>2</sup>), and normal coordinates:

75			
A			
Frequencies --	44.3399	78.4902	152.2659
Red. masses --	2.5612	3.2379	2.4147
Frc consts --	0.0030	0.0118	0.0330
IR Inten --	0.0199	0.8542	0.4908
Raman Activ --	4.7879	0.3468	1.0633
Depolar (P) --	0.7149	0.6609	0.5215
Depolar (U) --	0.8337	0.7958	0.6855
Dip. str. --	1.7930	43.4150	12.8596
Rot. str. --	0.4084	-0.1490	-4.0649
72			
A			
Frequencies --	176.3376	183.8388	205.4022
Red. masses --	2.1469	1.1790	1.3460
Frc consts --	0.0393	0.0235	0.0335
IR Inten --	0.1723	0.4439	0.3555
Raman Activ --	1.5497	0.2500	1.2507
Depolar (P) --	0.6906	0.7248	0.4972
Depolar (U) --	0.8170	0.8405	0.6642
Dip. str. --	3.8987	9.6339	6.9053
Rot. str. --	1.9851	-1.8977	-4.3990
69			
A			
Frequencies --	242.5618	263.7276	322.0328
Red. masses --	1.8334	3.5051	2.4862
Frc consts --	0.0636	0.1436	0.1519
IR Inten --	0.5319	0.9666	0.4697
Raman Activ --	1.2271	1.3954	1.7597
Depolar (P) --	0.4658	0.2076	0.5830
Depolar (U) --	0.6355	0.3438	0.7366
Dip. str. --	8.7477	14.6210	5.8181
Rot. str. --	0.4446	3.8799	-0.0523
66			
A			
Frequencies --	335.0556	403.8537	413.5084
Red. masses --	2.2613	3.2377	2.4619
Frc consts --	0.1496	0.3111	0.2480
IR Inten --	0.5342	8.9266	2.8860
Raman Activ --	2.7904	1.2015	0.3650
Depolar (P) --	0.4674	0.7342	0.7329

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Depolar (U) --	0.6370	0.8467	0.8459
Dip. str. --	6.3602	88.1800	27.8434
Rot. str. --	1.1889	1.1770	5.5367
	63	62	61
	A	A	A
Frequencies --	468.3131	504.3282	537.2289
Red. masses --	2.3779	2.3675	2.7890
Frc consts --	0.3073	0.3548	0.4743
IR Inten --	2.1602	2.5939	4.8973
Raman Activ --	0.9852	3.4325	2.9469
Depolar (P) --	0.5174	0.2570	0.7494
Depolar (U) --	0.6819	0.4090	0.8567
Dip. str. --	18.4022	20.5189	36.3664
Rot. str. --	4.3230	9.6817	35.8176
	60	59	58
	A	A	A
Frequencies --	563.0603	637.4240	691.7206
Red. masses --	3.1011	3.6544	4.0087
Frc consts --	0.5793	0.8748	1.1301
IR Inten --	5.3865	0.2974	4.5680
Raman Activ --	1.8134	1.1828	12.9797
Depolar (P) --	0.7000	0.7498	0.1561
Depolar (U) --	0.8235	0.8570	0.2701
Dip. str. --	38.1644	1.8616	26.3452
Rot. str. --	-24.2164	-1.7780	-8.9203
	57	56	55
	A	A	A
Frequencies --	729.4548	775.0722	798.8494
Red. masses --	1.1499	3.5911	1.7280
Frc consts --	0.3605	1.2710	0.6497
IR Inten --	0.6053	12.2126	1.7916
Raman Activ --	3.3719	8.5160	7.3552
Depolar (P) --	0.6402	0.3669	0.1720
Depolar (U) --	0.7806	0.5369	0.2935
Dip. str. --	3.3106	62.8596	8.9469
Rot. str. --	-5.5859	-11.5224	-17.9866
	54	53	52
	A	A	A
Frequencies --	861.3084	889.0284	911.2981
Red. masses --	2.3246	2.4587	1.9759
Frc consts --	1.0160	1.1450	0.9668
IR Inten --	10.6419	2.9530	4.2588
Raman Activ --	3.7474	1.6722	3.0287
Depolar (P) --	0.3273	0.7105	0.3525
Depolar (U) --	0.4932	0.8307	0.5213
Dip. str. --	49.2909	13.2511	18.6437
Rot. str. --	-10.5487	-7.1934	4.5505
	51	50	49
	A	A	A
Frequencies --	923.1458	934.5593	964.7217
Red. masses --	1.3537	1.7506	2.3511
Frc consts --	0.6797	0.9009	1.2892
IR Inten --	31.1585	0.5647	7.6563
Raman Activ --	0.6564	2.7000	1.9797
Depolar (P) --	0.6145	0.6272	0.5039
Depolar (U) --	0.7613	0.7709	0.6701
Dip. str. --	134.6520	2.4107	31.6609
Rot. str. --	40.5397	-4.2120	4.5628
	48	47	46
	A	A	A
Frequencies --	991.4750	1022.1258	1025.6687
Red. masses --	1.4009	1.7934	1.5770
Frc consts --	0.8114	1.1039	0.9774
IR Inten --	1.7382	2.0208	3.8979
Raman Activ --	0.8556	6.3606	4.3213
Depolar (P) --	0.7451	0.1814	0.6414
Depolar (U) --	0.8539	0.3071	0.7815
Dip. str. --	6.9939	7.8871	15.1611
Rot. str. --	-13.8681	-5.5085	38.8736
	45	44	43
	A	A	A
Frequencies --	1049.3804	1055.7343	1059.3687
Red. masses --	1.4829	1.5220	1.6779
Frc consts --	0.9621	0.9995	1.1095
IR Inten --	4.2584	2.9197	4.1477
Raman Activ --	2.5892	3.0555	5.8500
Depolar (P) --	0.7228	0.7351	0.7447
Depolar (U) --	0.8391	0.8473	0.8536
Dip. str. --	16.1891	11.0328	15.6197
Rot. str. --	-10.6080	30.6018	-2.8810
	42	41	40
	A	A	A
Frequencies --	1072.2565	1113.1006	1132.0021
Red. masses --	1.9798	2.4576	2.2426
Frc consts --	1.3411	1.7940	1.6932
IR Inten --	6.8009	0.1340	13.6313
Raman Activ --	4.9249	2.8175	2.6449
Depolar (P) --	0.7493	0.6992	0.5740
Depolar (U) --	0.8567	0.8229	0.7294
Dip. str. --	25.3031	0.4803	48.0394
Rot. str. --	-8.0158	-3.1404	15.9499
	39	38	37
	A	A	A
Frequencies --	1198.6424	1211.9734	1245.5159
Red. masses --	1.4610	1.4640	1.5632
Frc consts --	1.2368	1.2670	1.4288
IR Inten --	13.5432	3.4262	5.7633
Raman Activ --	3.2632	1.9774	0.8461
Depolar (P) --	0.5178	0.6453	0.6855
Depolar (U) --	0.6823	0.7844	0.8134
Dip. str. --	45.0753	11.2780	18.4600
Rot. str. --	16.6264	9.3203	-11.5973
	36	35	34
	A	A	A
Frequencies --	1273.0781	1292.9944	1303.0487
Red. masses --	1.4383	1.9294	1.5388
Frc consts --	1.3735	1.9005	1.5394

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IR Inten	--	3.5952	5.6732	0.9513
Raman Activ	--	8.8525	2.2813	7.2348
Depolar (P)	--	0.5921	0.6432	0.5261
Depolar (U)	--	0.7438	0.7829	0.6895
Dip. str.	--	11.2662	17.5040	2.9126
Rot. str.	--	11.7808	-0.2001	-3.3258
		33	32	31
		A	A	A
Frequencies	--	1316.9964	1326.2382	1369.3983
Red. masses	--	1.3639	1.3350	1.4045
Frc const	--	1.3938	1.3835	1.5518
IR Inten	--	4.0434	1.7626	1.9646
Raman Activ	--	11.8233	2.5089	8.2469
Depolar (P)	--	0.6581	0.2609	0.4466
Depolar (U)	--	0.7938	0.4139	0.6174
Dip. str.	--	12.2480	5.3021	5.7234
Rot. str.	--	-23.3030	11.8301	-3.2157
		30	29	28
		A	A	A
Frequencies	--	1374.1427	1386.0412	1396.1178
Red. masses	--	1.6508	1.4780	1.3787
Frc const	--	1.8365	1.6729	1.5833
IR Inten	--	0.3062	2.6369	3.9568
Raman Activ	--	5.7434	5.5269	1.9485
Depolar (P)	--	0.6807	0.7495	0.4825
Depolar (U)	--	0.8100	0.8568	0.6509
Dip. str.	--	0.8889	7.5896	11.3066
Rot. str.	--	-8.8671	5.1831	6.5582
		27	26	25
		A	A	A
Frequencies	--	1398.2577	1430.5348	1443.4059
Red. masses	--	1.4053	1.1817	1.2091
Frc const	--	1.6188	1.4248	1.4842
IR Inten	--	9.7945	0.3053	2.7903
Raman Activ	--	6.8485	22.0980	21.8712
Depolar (P)	--	0.7492	0.4583	0.6992
Depolar (U)	--	0.8566	0.6285	0.8230
Dip. str.	--	27.9450	0.8515	7.7119
Rot. str.	--	-9.8596	1.8564	-2.6714
		24	23	22
		A	A	A
Frequencies	--	1448.9371	1451.0447	1452.7049
Red. masses	--	1.0788	1.1106	1.0511
Frc const	--	1.3344	1.3778	1.3069
IR Inten	--	5.4484	2.6810	4.9765
Raman Activ	--	18.0904	2.1366	6.1447
Depolar (P)	--	0.7327	0.6928	0.7454
Depolar (U)	--	0.8458	0.8185	0.8541
Dip. str.	--	15.0011	7.3711	13.6664
Rot. str.	--	3.4025	-1.2118	13.7567
		21	20	19
		A	A	A
Frequencies	--	1461.9776	1467.3134	1471.7791
Red. masses	--	1.0663	1.0707	1.0927
Frc const	--	1.3428	1.3582	1.3945
IR Inten	--	6.3357	9.7972	2.6343
Raman Activ	--	14.2923	3.7927	6.9112
Depolar (P)	--	0.7493	0.6417	0.7381
Depolar (U)	--	0.8567	0.7817	0.8493
Dip. str.	--	17.2887	26.6371	7.1406
Rot. str.	--	7.0132	7.5517	0.5205
		18	17	16
		A	A	A
Frequencies	--	1494.4407	1714.8916	3013.5385
Red. masses	--	2.5587	5.5637	1.0628
Frc const	--	3.3669	9.6402	5.6866
IR Inten	--	7.8232	19.3710	11.7725
Raman Activ	--	2.1921	28.8451	29.1780
Depolar (P)	--	0.0916	0.1656	0.4228
Depolar (U)	--	0.1678	0.2841	0.5944
Dip. str.	--	20.8841	45.0633	15.5847
Rot. str.	--	-7.0750	1.6262	7.3674
		15	14	13
		A	A	A
Frequencies	--	3016.9463	3023.1660	3024.3821
Red. masses	--	1.0568	1.0500	1.0440
Frc const	--	5.6676	5.6540	5.6262
IR Inten	--	15.5272	13.5262	31.6043
Raman Activ	--	42.8282	34.4625	148.4952
Depolar (P)	--	0.7414	0.0654	0.0621
Depolar (U)	--	0.8515	0.1228	0.1169
Dip. str.	--	20.5321	17.8492	41.6885
Rot. str.	--	-24.3921	-16.5070	-1.7231
		12	11	10
		A	A	A
Frequencies	--	3027.9236	3045.5211	3060.3816
Red. masses	--	1.0498	1.0853	1.0976
Frc const	--	5.6707	5.9311	6.0570
IR Inten	--	41.8896	3.7831	49.0529
Raman Activ	--	276.5289	49.3444	17.8511
Depolar (P)	--	0.0392	0.7461	0.6520
Depolar (U)	--	0.0754	0.8546	0.7894
Dip. str.	--	55.1910	4.9556	63.9434
Rot. str.	--	15.7159	7.0544	26.6345
		9	8	7
		A	A	A
Frequencies	--	3064.4091	3073.9345	3075.7331
Red. masses	--	1.0988	1.1018	1.0994
Frc const	--	6.0794	6.1341	6.1280
IR Inten	--	7.6735	39.6888	12.3498
Raman Activ	--	125.4564	47.4916	92.4431
Depolar (P)	--	0.3342	0.3591	0.7495
Depolar (U)	--	0.5010	0.5285	0.8568
Dip. str.	--	9.9898	51.5087	16.0184
Rot. str.	--	17.0255	-60.2276	37.5069
		6	5	4
		A	A	A

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Frequencies	--	3077.3040	3092.3174	3115.3118
Red. masses	--	1.0890	1.1010	1.1002
Frc consts	--	6.0763	6.2029	6.2912
IR Inten	--	58.4609	24.4030	23.1267
Raman Activ	--	143.6895	83.9913	73.1280
Depolar (P)	--	0.1797	0.7498	0.6915
Depolar (U)	--	0.3047	0.8570	0.8176
Dip. str.	--	75.7884	31.4823	29.6155
Rot. str.	--	-5.2053	18.2627	6.5112
		3	2	1
		A	A	A
Frequencies	--	3121.2007	3130.0114	3220.3004
Red. masses	--	1.1016	1.0608	1.1157
Frc consts	--	6.3229	6.1229	6.8171
IR Inten	--	20.0228	10.3560	19.1961
Raman Activ	--	78.4216	145.8674	89.9499
Depolar (P)	--	0.7028	0.1319	0.7265
Depolar (U)	--	0.8255	0.2330	0.8416
Dip. str.	--	25.5924	13.1994	23.7807
Rot. str.	--	-7.2698	-8.9164	-15.3010

## S-(-)-Limonene Oxide, eq-c255 (2.5 kJ/mol)

Harmonic frequencies (cm<sup>-1</sup>), IR intensities (KM/Mole), Raman scattering activities (A<sup>4</sup>/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), Dipole strengths (10<sup>-40</sup> esu<sup>2</sup>-cm<sup>2</sup>), Rotational strengths (10<sup>-44</sup> esu<sup>2</sup>-cm<sup>2</sup>), and normal coordinates:

		75	74	73
		A	A	A
Frequencies	--	44.0444	79.7881	153.0002
Red. masses	--	2.6118	3.2551	1.9599
Frc consts	--	0.0030	0.0122	0.0270
IR Inten	--	0.6377	1.3461	0.3610
Raman Activ	--	3.1793	0.5401	0.2184
Depolar (P)	--	0.7486	0.7393	0.7498
Depolar (U)	--	0.8562	0.8501	0.8570
Dip. str.	--	57.7652	67.3055	9.4135
Rot. str.	--	-3.3761	1.2514	-3.4471
		72	71	70
		A	A	A
Frequencies	--	180.2275	188.6678	205.7677
Red. masses	--	1.2725	2.3382	1.2887
Frc consts	--	0.0244	0.0490	0.0321
IR Inten	--	0.3677	0.1125	0.2586
Raman Activ	--	0.5209	0.6180	0.5713
Depolar (P)	--	0.7074	0.7494	0.6608
Depolar (U)	--	0.8287	0.8567	0.7957
Dip. str.	--	8.1397	2.3782	5.0130
Rot. str.	--	-1.5560	-0.9988	-5.9437
		69	68	67
		A	A	A
Frequencies	--	246.3549	283.3702	318.1781
Red. masses	--	1.8744	4.1338	2.4571
Frc consts	--	0.0670	0.1956	0.1466
IR Inten	--	0.4821	0.5187	0.1696
Raman Activ	--	0.6757	3.5178	0.7488
Depolar (P)	--	0.7097	0.2862	0.7386
Depolar (U)	--	0.8302	0.4450	0.8497
Dip. str.	--	7.8077	7.3020	2.1260
Rot. str.	--	3.7496	-0.2223	0.2768
		66	65	64
		A	A	A
Frequencies	--	342.1417	406.5826	419.5885
Red. masses	--	2.2576	2.8495	2.6437
Frc consts	--	0.1557	0.2775	0.2742
IR Inten	--	1.4545	7.3353	5.4873
Raman Activ	--	0.8884	0.7562	0.7887
Depolar (P)	--	0.7439	0.5976	0.5840
Depolar (U)	--	0.8532	0.7482	0.7374
Dip. str.	--	16.9590	71.9741	52.1725
Rot. str.	--	4.0934	6.2085	5.9365
		63	62	61
		A	A	A
Frequencies	--	444.0683	497.5394	546.7137
Red. masses	--	2.4608	2.5234	2.2498
Frc consts	--	0.2859	0.3680	0.3962
IR Inten	--	0.3357	1.0489	4.8405
Raman Activ	--	0.7702	2.3883	3.2031
Depolar (P)	--	0.6157	0.3677	0.3495
Depolar (U)	--	0.7621	0.5377	0.5180
Dip. str.	--	3.0155	8.4102	35.3212
Rot. str.	--	-0.5969	-2.2627	-2.7824
		60	59	58
		A	A	A
Frequencies	--	555.9719	638.5362	693.7841
Red. masses	--	3.5398	3.7213	4.1144
Frc consts	--	0.6447	0.8940	1.1668
IR Inten	--	6.9627	0.3744	5.0691
Raman Activ	--	1.6122	1.3448	13.0352
Depolar (P)	--	0.5157	0.7199	0.1714
Depolar (U)	--	0.6805	0.8372	0.2927
Dip. str.	--	49.9609	2.3389	29.1484
Rot. str.	--	12.3883	-0.1470	-5.7963
		57	56	55
		A	A	A
Frequencies	--	713.7045	776.6650	810.6753
Red. masses	--	1.1723	3.1936	1.6121
Frc consts	--	0.3518	1.1350	0.6242
IR Inten	--	0.3161	13.5013	2.1590
Raman Activ	--	6.8667	6.5301	1.8697
Depolar (P)	--	0.3766	0.4295	0.1931
Depolar (U)	--	0.5471	0.6009	0.3236

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Dip. str.	--	1.7670	69.3502	10.6246
Rot. str.	--	-11.1810	-6.6003	-17.6916
		54	53	52
		A	A	A
Frequencies	--	864.7297	897.3879	915.3217
Red. masses	--	2.3802	2.2511	1.6871
Frc const	--	1.0486	1.0681	0.8328
IR Inten	--	9.8741	1.5735	14.8223
Raman Activ	--	5.6427	1.3981	2.4214
Depolar (P)	--	0.2276	0.5339	0.2478
Depolar (U)	--	0.3708	0.6961	0.3971
Dip. str.	--	45.5539	6.9952	64.6025
Rot. str.	--	-20.0523	3.3191	18.7729
		51	50	49
		A	A	A
Frequencies	--	920.1593	934.8356	965.6176
Red. masses	--	1.6783	1.7924	2.0681
Frc const	--	0.8372	0.9229	1.1361
IR Inten	--	19.5547	1.2530	5.6214
Raman Activ	--	1.8241	1.6082	1.2713
Depolar (P)	--	0.1522	0.7422	0.6530
Depolar (U)	--	0.2643	0.8520	0.7901
Dip. str.	--	84.7802	5.3471	23.2247
Rot. str.	--	-30.9814	-10.5235	3.5379
		48	47	46
		A	A	A
Frequencies	--	989.4677	1008.1970	1033.4960
Red. masses	--	1.7705	1.6810	1.4905
Frc const	--	1.0213	1.0067	0.9380
IR Inten	--	3.6430	0.3308	4.0870
Raman Activ	--	2.2563	1.7323	3.0725
Depolar (P)	--	0.4408	0.7500	0.3917
Depolar (U)	--	0.6119	0.8571	0.5629
Dip. str.	--	14.6879	1.3091	15.7763
Rot. str.	--	-11.6769	-9.1901	27.6795
		45	44	43
		A	A	A
Frequencies	--	1049.8516	1051.3728	1061.8857
Red. masses	--	1.6461	1.5604	1.4503
Frc const	--	1.0689	1.0162	0.9635
IR Inten	--	0.9545	6.0860	2.6045
Raman Activ	--	1.4306	2.7344	10.3332
Depolar (P)	--	0.5762	0.6891	0.7270
Depolar (U)	--	0.7312	0.8159	0.8419
Dip. str.	--	3.6271	23.0932	9.7850
Rot. str.	--	4.0611	2.5532	6.7053
		42	41	40
		A	A	A
Frequencies	--	1070.6803	1121.5541	1133.4263
Red. masses	--	2.0307	2.2941	2.3141
Frc const	--	1.3715	1.7002	1.7515
IR Inten	--	5.6218	2.4219	10.5028
Raman Activ	--	3.6062	1.3581	3.1119
Depolar (P)	--	0.6510	0.7278	0.4052
Depolar (U)	--	0.7886	0.8424	0.5767
Dip. str.	--	20.9472	8.6148	36.9674
Rot. str.	--	26.3766	0.5199	5.5769
		39	38	37
		A	A	A
Frequencies	--	1196.3524	1211.1076	1233.9971
Red. masses	--	1.4414	1.4375	1.6924
Frc const	--	1.2155	1.2423	1.5184
IR Inten	--	7.5025	0.6571	14.8907
Raman Activ	--	3.5014	1.7318	2.3633
Depolar (P)	--	0.2763	0.4554	0.7495
Depolar (U)	--	0.4330	0.6258	0.8568
Dip. str.	--	25.0180	2.1646	48.1402
Rot. str.	--	27.4752	-3.2272	-15.4317
		36	35	34
		A	A	A
Frequencies	--	1269.7040	1276.0041	1305.7210
Red. masses	--	1.5570	1.5000	1.4675
Frc const	--	1.4789	1.4389	1.4741
IR Inten	--	3.6591	2.9934	6.6912
Raman Activ	--	3.7875	4.3710	5.6223
Depolar (P)	--	0.5912	0.6440	0.6284
Depolar (U)	--	0.7431	0.7835	0.7718
Dip. str.	--	11.4968	9.3587	20.4438
Rot. str.	--	2.5995	7.4121	21.9542
		33	32	31
		A	A	A
Frequencies	--	1315.0955	1337.8556	1360.4915
Red. masses	--	1.3226	1.4158	1.5114
Frc const	--	1.3476	1.4930	1.6482
IR Inten	--	2.8477	0.6926	1.0226
Raman Activ	--	11.9623	2.4061	4.1182
Depolar (P)	--	0.6135	0.7475	0.5046
Depolar (U)	--	0.7605	0.8555	0.6707
Dip. str.	--	8.6387	2.0653	2.9986
Rot. str.	--	-22.0110	7.9879	9.5114
		30	29	28
		A	A	A
Frequencies	--	1377.1460	1393.7047	1396.8416
Red. masses	--	1.6873	1.2715	1.3906
Frc const	--	1.8854	1.4551	1.5987
IR Inten	--	1.6820	3.2581	7.4320
Raman Activ	--	2.5427	5.3607	3.5829
Depolar (P)	--	0.4503	0.6058	0.6715
Depolar (U)	--	0.6209	0.7545	0.8035
Dip. str.	--	4.8725	9.3260	21.2260
Rot. str.	--	-14.5021	-5.9035	6.4335
		27	26	25
		A	A	A
Frequencies	--	1406.6020	1428.8761	1443.6449
Red. masses	--	1.6743	1.1770	1.2170
Frc const	--	1.9517	1.4159	1.4943
IR Inten	--	1.7135	0.3733	3.9906

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Raman Activ	--	5.4880	32.7858	15.4267
Depolar (P)	--	0.5926	0.5950	0.6180
Depolar (U)	--	0.7442	0.7461	0.7639
Dip. str.	--	4.8599	1.0423	11.0276
Rot. str.	--	-6.1103	0.3662	-4.8185
		24	23	22
		A	A	A
Frequencies	--	1448.6018	1451.0010	1451.4133
Red. masses	--	1.0785	1.0711	1.0825
Frc consts	--	1.3334	1.3286	1.3436
IR Inten	--	0.9730	4.2371	5.7335
Raman Activ	--	5.3600	11.1335	8.6789
Depolar (P)	--	0.7469	0.7500	0.7462
Depolar (U)	--	0.8551	0.8571	0.8547
Dip. str.	--	2.6796	11.6495	15.7593
Rot. str.	--	1.2183	0.7934	2.1473
		21	20	19
		A	A	A
Frequencies	--	1462.0327	1466.4739	1474.1436
Red. masses	--	1.0649	1.0689	1.0968
Frc consts	--	1.3411	1.3543	1.4043
IR Inten	--	6.4440	15.8947	0.9981
Raman Activ	--	13.6765	5.4835	4.4709
Depolar (P)	--	0.7497	0.6872	0.7293
Depolar (U)	--	0.8570	0.8146	0.8434
Dip. str.	--	17.5836	43.2399	2.7011
Rot. str.	--	7.4355	-3.4367	0.0526
		18	17	16
		A	A	A
Frequencies	--	1496.0552	1716.2350	3007.9528
Red. masses	--	2.6169	5.4499	1.0755
Frc consts	--	3.4509	9.4578	5.7333
IR Inten	--	10.0949	20.6702	1.6839
Raman Activ	--	2.0841	22.6868	86.3627
Depolar (P)	--	0.0887	0.1312	0.2572
Depolar (U)	--	0.1630	0.2319	0.4092
Dip. str.	--	26.9193	48.0480	2.2334
Rot. str.	--	-8.0477	7.2440	0.2476
		15	14	13
		A	A	A
Frequencies	--	3015.1157	3018.7319	3022.3784
Red. masses	--	1.0589	1.0461	1.0662
Frc consts	--	5.6718	5.6164	5.7383
IR Inten	--	2.8183	31.0121	40.5401
Raman Activ	--	30.9824	176.2870	21.3731
Depolar (P)	--	0.2224	0.0331	0.0729
Depolar (U)	--	0.3639	0.0642	0.1359
Dip. str.	--	3.7290	40.9839	53.5110
Rot. str.	--	13.2933	-33.2878	6.4051
		12	11	10
		A	A	A
Frequencies	--	3023.1729	3027.8515	3062.1465
Red. masses	--	1.0530	1.0475	1.1010
Frc consts	--	5.6702	5.6584	6.0826
IR Inten	--	4.8387	42.1691	30.2779
Raman Activ	--	16.0279	242.9506	57.0751
Depolar (P)	--	0.6940	0.0369	0.5877
Depolar (U)	--	0.8194	0.0712	0.7403
Dip. str.	--	6.3852	55.5606	39.4463
Rot. str.	--	-17.0422	34.5895	-18.8704
		9	8	7
		A	A	A
Frequencies	--	3065.9975	3071.8283	3077.0676
Red. masses	--	1.0972	1.0981	1.1008
Frc consts	--	6.0770	6.1049	6.1411
IR Inten	--	26.1005	16.3901	25.9635
Raman Activ	--	80.8819	82.0098	96.4606
Depolar (P)	--	0.4023	0.7317	0.3959
Depolar (U)	--	0.5738	0.8451	0.5672
Dip. str.	--	33.9613	21.2858	33.6615
Rot. str.	--	47.2392	16.3938	-29.0539
		6	5	4
		A	A	A
Frequencies	--	3077.4192	3092.6324	3115.3790
Red. masses	--	1.0893	1.1010	1.1006
Frc consts	--	6.0782	6.2041	6.2934
IR Inten	--	63.5530	23.9894	23.8293
Raman Activ	--	145.9626	83.2318	75.2909
Depolar (P)	--	0.1571	0.7500	0.6866
Depolar (U)	--	0.2716	0.8571	0.8142
Dip. str.	--	82.3866	30.9456	30.5146
Rot. str.	--	-13.5700	18.5325	-7.7055
		3	2	1
		A	A	A
Frequencies	--	3121.2771	3142.6576	3231.3042
Red. masses	--	1.1016	1.0615	1.1141
Frc consts	--	6.3234	6.1767	6.8538
IR Inten	--	19.8511	9.1393	17.1848
Raman Activ	--	77.6642	145.3030	67.4799
Depolar (P)	--	0.7003	0.1530	0.7478
Depolar (U)	--	0.8238	0.2654	0.8557
Dip. str.	--	25.3723	11.6017	21.2165
Rot. str.	--	-7.3700	0.0917	7.1990

S-(-)-Limonene Oxide, eq-c305 (2.8 kJ/mol)

Harmonic frequencies (cm<sup>-1</sup>), IR intensities (KM/Mole), Raman scattering activities (A<sup>4</sup>/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), Dipole strengths (10<sup>-40</sup> esu<sup>2</sup>-cm<sup>2</sup>), Rotational strengths (10<sup>-44</sup> esu<sup>2</sup>-cm<sup>2</sup>),



and normal coordinates:

	75	74	73
	A	A	A
Frequencies --	34.8221	77.0407	144.4515
Red. masses --	2.5736	3.2880	2.0892
Frc consts --	0.0018	0.0115	0.0257
IR Inten --	0.7523	4.5311	0.3887
Raman Activ --	3.2264	0.4152	0.1629
Depolar (P) --	0.7488	0.7341	0.7463
Depolar (U) --	0.8563	0.8467	0.8547
Dip. str. --	86.1858	234.6325	10.7361
Rot. str. --	5.0190	3.3025	-5.2066
	72	71	70
	A	A	A
Frequencies --	169.0916	187.8337	209.9540
Red. masses --	1.4317	1.5458	1.4547
Frc consts --	0.0241	0.0321	0.0378
IR Inten --	0.6017	0.7206	1.1468
Raman Activ --	0.3874	0.8916	0.2605
Depolar (P) --	0.7322	0.7432	0.6508
Depolar (U) --	0.8454	0.8527	0.7885
Dip. str. --	14.1964	15.3053	21.7901
Rot. str. --	-5.7976	16.5871	-4.8466
	69	68	67
	A	A	A
Frequencies --	243.1210	289.8564	322.3930
Red. masses --	1.9827	4.1261	2.5023
Frc consts --	0.0690	0.2042	0.1532
IR Inten --	0.7441	0.7262	0.6940
Raman Activ --	0.2004	3.7498	0.2973
Depolar (P) --	0.3410	0.2772	0.7486
Depolar (U) --	0.5085	0.4341	0.8562
Dip. str. --	12.2094	9.9944	8.5879
Rot. str. --	1.4321	3.5908	-1.7168
	66	65	64
	A	A	A
Frequencies --	331.8996	398.3074	411.7830
Red. masses --	2.1610	3.5216	2.2560
Frc consts --	0.1403	0.3292	0.2254
IR Inten --	0.8764	9.6142	4.2177
Raman Activ --	1.4367	1.1696	0.1916
Depolar (P) --	0.7464	0.7475	0.7484
Depolar (U) --	0.8548	0.8555	0.8561
Dip. str. --	10.5338	96.2950	40.8617
Rot. str. --	-1.2798	4.0187	0.2433
	63	62	61
	A	A	A
Frequencies --	451.5144	502.0443	528.1824
Red. masses --	2.4230	2.4939	2.4068
Frc consts --	0.2910	0.3703	0.3956
IR Inten --	0.1351	3.3572	7.8781
Raman Activ --	1.2052	2.0683	3.2919
Depolar (P) --	0.7001	0.4636	0.4253
Depolar (U) --	0.8236	0.6335	0.5968
Dip. str. --	1.1940	26.6773	59.5036
Rot. str. --	1.2852	1.4021	-3.3077
	60	59	58
	A	A	A
Frequencies --	569.7985	637.5537	690.0071
Red. masses --	3.0498	3.7440	3.1321
Frc consts --	0.5834	0.8966	0.8786
IR Inten --	4.9837	0.8796	5.7309
Raman Activ --	1.6206	1.4852	13.3992
Depolar (P) --	0.3228	0.6943	0.1341
Depolar (U) --	0.4880	0.8196	0.2365
Dip. str. --	34.8928	5.5041	33.1344
Rot. str. --	14.2340	-0.7846	28.4214
	57	56	55
	A	A	A
Frequencies --	700.1869	775.1929	802.9622
Red. masses --	1.2619	3.7540	1.6081
Frc consts --	0.3645	1.3291	0.6109
IR Inten --	22.6300	14.1817	0.2562
Raman Activ --	3.5280	8.3152	3.8614
Depolar (P) --	0.7389	0.4146	0.2442
Depolar (U) --	0.8498	0.5862	0.3925
Dip. str. --	128.9372	72.9835	1.2729
Rot. str. --	-48.6355	-16.9325	-2.8594
	54	53	52
	A	A	A
Frequencies --	866.7912	901.9200	916.5524
Red. masses --	2.3943	2.3043	1.9370
Frc consts --	1.0599	1.1044	0.9587
IR Inten --	11.1928	3.5253	16.7235
Raman Activ --	3.8603	1.2996	3.1227
Depolar (P) --	0.1581	0.3974	0.2167
Depolar (U) --	0.2730	0.5688	0.3563
Dip. str. --	51.5147	15.5932	72.7909
Rot. str. --	-39.5195	-10.2549	44.9390
	51	50	49
	A	A	A
Frequencies --	918.6325	933.6437	963.2980
Red. masses --	1.4451	1.7796	2.2300
Frc consts --	0.7185	0.9140	1.2192
IR Inten --	15.5646	2.7323	3.8162
Raman Activ --	1.2040	1.7828	2.1448
Depolar (P) --	0.3216	0.6873	0.7358
Depolar (U) --	0.4867	0.8147	0.8478
Dip. str. --	67.5932	11.6748	15.8045
Rot. str. --	-26.1601	-4.8935	-5.7660
	48	47	46
	A	A	A
Frequencies --	998.1372	1011.8623	1029.2501
Red. masses --	1.9863	1.4360	1.6255
Frc consts --	1.1659	0.8662	1.0145
IR Inten --	6.2897	4.8015	2.7869
Raman Activ --	1.1761	5.2886	1.5948

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Depolar (P) --	0.1830	0.5220	0.4733
Depolar (U) --	0.3094	0.6859	0.6425
Dip. str. --	25.1388	18.9305	10.8020
Rot. str. --	-8.2775	5.6469	-16.1496
	45	44	43
	A	A	A
Frequencies --	1048.7011	1058.4121	1066.9442
Red. masses --	1.5921	1.5252	1.6543
Frc consts --	1.0316	1.0066	1.1095
IR Inten --	4.7070	4.4116	2.7753
Raman Activ --	2.5541	5.4507	3.4172
Depolar (P) --	0.7458	0.7161	0.7140
Depolar (U) --	0.8544	0.8346	0.8332
Dip. str. --	17.9061	16.6282	10.3771
Rot. str. --	9.3775	4.2400	13.1263
	42	41	40
	A	A	A
Frequencies --	1083.9695	1115.6914	1136.1357
Red. masses --	1.7672	2.3392	2.2823
Frc consts --	1.2234	1.7155	1.7358
IR Inten --	3.7492	0.6935	15.1442
Raman Activ --	1.5318	3.0151	3.4156
Depolar (P) --	0.5073	0.7071	0.4837
Depolar (U) --	0.6731	0.8284	0.6520
Dip. str. --	13.7985	2.4797	53.1769
Rot. str. --	22.0034	-8.4243	25.9563
	39	38	37
	A	A	A
Frequencies --	1199.8243	1211.6166	1229.1009
Red. masses --	1.4634	1.4627	1.6302
Frc consts --	1.2413	1.2651	1.4510
IR Inten --	6.9538	2.5441	5.2765
Raman Activ --	2.9303	5.0446	0.2822
Depolar (P) --	0.4140	0.4323	0.6706
Depolar (U) --	0.5855	0.6037	0.8028
Dip. str. --	23.1213	8.3769	17.1265
Rot. str. --	11.8976	0.6111	-5.6695
	36	35	34
	A	A	A
Frequencies --	1260.5529	1283.3504	1311.1811
Red. masses --	1.5862	1.3466	1.4942
Frc consts --	1.4850	1.3067	1.5135
IR Inten --	5.8911	0.6443	4.9375
Raman Activ --	4.0421	6.9770	10.0269
Depolar (P) --	0.5066	0.7340	0.5682
Depolar (U) --	0.6725	0.8466	0.7247
Dip. str. --	18.6441	2.0028	15.0228
Rot. str. --	4.9078	3.6039	-21.3120
	33	32	31
	A	A	A
Frequencies --	1318.9562	1329.4579	1363.0477
Red. masses --	1.3882	1.4622	1.3974
Frc consts --	1.4228	1.5226	1.5296
IR Inten --	0.6885	2.9372	2.7741
Raman Activ --	3.8863	1.1952	7.2226
Depolar (P) --	0.7500	0.5653	0.7488
Depolar (U) --	0.8571	0.7223	0.8564
Dip. str. --	2.0826	8.8139	8.1192
Rot. str. --	4.1161	1.0327	-21.4328
	30	29	28
	A	A	A
Frequencies --	1379.1726	1393.4993	1396.4228
Red. masses --	1.6757	1.3344	1.3700
Frc consts --	1.8779	1.5266	1.5740
IR Inten --	1.3205	7.3709	1.2792
Raman Activ --	3.1318	3.4920	4.6851
Depolar (P) --	0.3697	0.6314	0.6086
Depolar (U) --	0.5399	0.7740	0.7567
Dip. str. --	3.8196	21.1018	3.6544
Rot. str. --	1.1278	4.7213	-1.9575
	27	26	25
	A	A	A
Frequencies --	1406.2290	1425.2576	1443.0193
Red. masses --	1.7841	1.1590	1.1645
Frc consts --	2.0786	1.3871	1.4287
IR Inten --	1.3758	7.9114	3.6029
Raman Activ --	5.2517	27.4117	16.1526
Depolar (P) --	0.5453	0.5637	0.7100
Depolar (U) --	0.7057	0.7209	0.8304
Dip. str. --	3.9029	22.1447	9.9606
Rot. str. --	17.9449	-7.6041	0.5798
	24	23	22
	A	A	A
Frequencies --	1449.0633	1450.9541	1452.6676
Red. masses --	1.0948	1.1008	1.0703
Frc consts --	1.3544	1.3655	1.3307
IR Inten --	0.7292	9.8070	2.8079
Raman Activ --	11.8732	3.5691	5.2949
Depolar (P) --	0.7241	0.7415	0.7266
Depolar (U) --	0.8400	0.8516	0.8416
Dip. str. --	2.0075	26.9644	7.7113
Rot. str. --	-2.7575	-2.3570	6.2426
	21	20	19
	A	A	A
Frequencies --	1460.5946	1464.7964	1472.0446
Red. masses --	1.0661	1.0619	1.0950
Frc consts --	1.3400	1.3424	1.3980
IR Inten --	3.2969	17.3822	4.7096
Raman Activ --	16.6779	5.7498	9.3571
Depolar (P) --	0.7465	0.7203	0.7447
Depolar (U) --	0.8549	0.8374	0.8536
Dip. str. --	9.0050	47.3406	12.7635
Rot. str. --	-5.1419	-2.7111	12.0066
	18	17	16
	A	A	A
Frequencies --	1496.2223	1718.8614	3002.5379
Red. masses --	2.6187	5.2662	1.0593

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Frc consts	--	3.4540	9.1671	5.6266
IR Inten	--	9.0903	18.9833	16.2932
Raman Activ	--	2.7057	22.0925	21.5626
Depolar (P)	--	0.1167	0.1346	0.3648
Depolar (U)	--	0.2089	0.2372	0.5346
Dip. str.	--	24.2375	44.0594	21.6483
Rot. str.	--	-20.0607	-5.7115	-14.5929
		15	14	13
		A	A	A
Frequencies	--	3016.2065	3020.8624	3022.0070
Red. masses	--	1.0621	1.0585	1.0544
Frc consts	--	5.6932	5.6912	5.6736
IR Inten	--	17.7075	4.4010	15.6473
Raman Activ	--	69.3556	261.2784	11.2365
Depolar (P)	--	0.1503	0.0590	0.6050
Depolar (U)	--	0.2614	0.1115	0.7539
Dip. str.	--	23.4209	5.8120	20.6562
Rot. str.	--	13.5864	3.2516	-27.8355
		12	11	10
		A	A	A
Frequencies	--	3025.8837	3027.9803	3062.0639
Red. masses	--	1.0571	1.0549	1.1016
Frc consts	--	5.7025	5.6988	6.0857
IR Inten	--	48.4018	17.0843	26.1809
Raman Activ	--	112.2839	84.5352	63.0240
Depolar (P)	--	0.0505	0.0568	0.6851
Depolar (U)	--	0.0962	0.1076	0.8131
Dip. str.	--	63.8141	22.5087	34.1096
Rot. str.	--	35.0088	-20.5885	-6.4931
		9	8	7
		A	A	A
Frequencies	--	3064.5378	3073.8224	3077.4766
Red. masses	--	1.0971	1.0974	1.0996
Frc consts	--	6.0707	6.1092	6.1361
IR Inten	--	14.6318	29.8737	39.7243
Raman Activ	--	86.8353	89.5915	85.1628
Depolar (P)	--	0.3392	0.7185	0.3801
Depolar (U)	--	0.5065	0.8362	0.5508
Dip. str.	--	19.0477	38.7719	51.4955
Rot. str.	--	46.1238	20.5968	-21.5216
		6	5	4
		A	A	A
Frequencies	--	3079.2345	3092.6995	3114.4909
Red. masses	--	1.0889	1.1010	1.1010
Frc consts	--	6.0831	6.2044	6.2921
IR Inten	--	58.5169	24.6740	29.4855
Raman Activ	--	154.7436	78.9333	81.9964
Depolar (P)	--	0.1613	0.7496	0.6069
Depolar (U)	--	0.2778	0.8569	0.7554
Dip. str.	--	75.8134	31.8279	37.7684
Rot. str.	--	-18.6611	12.4921	18.2537
		3	2	1
		A	A	A
Frequencies	--	3121.4900	3143.1903	3231.8354
Red. masses	--	1.1014	1.0618	1.1132
Frc consts	--	6.3231	6.1809	6.8503
IR Inten	--	17.2436	11.5918	4.9518
Raman Activ	--	73.2986	133.9597	71.9870
Depolar (P)	--	0.7333	0.1470	0.7379
Depolar (U)	--	0.8462	0.2563	0.8492
Dip. str.	--	22.0380	14.7126	6.1126
Rot. str.	--	-6.9280	3.3810	5.8319

**Table 3S:** Output of the MolVib program for the five most stable equatorial conformers (eq-t110, eq-t255, eq-c110, eq-c255 and eq-c305) of the S-(-)-Limonene oxide

S-(-)-Limonene Oxide, eq-t110 (0.0 kJ/mol)										
NR.	75	74	73							
CALC.	54.0	65.1	165.1							
C-O	0.0	0.0	0.0							
OBS.	0.0	0.0	0.0							
IRINT.	0.579	0.913	0.283							
RACT.	5.030	0.815	1.082							
DEPOL.	0.749	0.742	0.735							
NR.	72	71	70	69	68	67	66	65	64	
CALC.	177.0	186.5	208.2	232.7	281.4	315.8	317.9	387.3	439.6	
C-O	-3.0	6.5	0.2	-12.3	-6.6	-6.2	-4.1	-5.7	-5.4	
OBS.	180.0	180.0	208.0	245.0	288.0	322.0	322.0	393.0	445.0	
IRINT.	0.165	0.357	0.839	0.921	0.845	1.472	0.221	5.030	6.081	
RACT.	0.641	0.224	0.478	0.336	2.173	1.306	2.005	0.934	0.743	
DEPOL.	0.716	0.702	0.660	0.242	0.296	0.664	0.629	0.604	0.362	
NR.	63	62	61	60	59	58	57	56	55	
CALC.	470.3	505.6	528.2	560.0	609.8	671.4	706.7	751.8	794.4	
C-O	1.3	0.6	-1.8	3.0	-1.2	-0.6	5.7	-4.2	-2.6	
OBS.	469.0	505.0	530.0	557.0	611.0	672.0	701.0	756.0	797.0	
IRINT.	0.194	5.588	2.555	6.796	0.435	5.537	0.645	8.677	3.784	
RACT.	0.731	3.830	3.302	1.352	1.788	9.068	3.444	14.867	2.453	
DEPOL.	0.739	0.100	0.577	0.665	0.749	0.169	0.489	0.189	0.527	
NR.	54	53	52	51	50	49	48	47	46	
CALC.	843.0	881.4	888.2	905.4	912.1	971.4	976.4	997.4	1010.8	
C-O	0.0	-5.6	1.2	0.4	-3.9	1.4	6.4	-0.6	-3.2	
OBS.	843.0	887.0	887.0	905.0	916.0	970.0	970.0	998.0	1014.0	
IRINT.	13.297	7.290	0.803	33.129	1.095	2.248	1.300	5.002	6.425	
RACT.	1.974	5.687	1.393	0.256	0.832	0.868	0.922	3.155	4.335	
DEPOL.	0.383	0.382	0.473	0.628	0.098	0.500	0.703	0.732	0.210	
NR.	45	44	43	42	41	40	39	38	37	
CALC.	1026.7	1036.5	1041.2	1082.4	1092.7	1114.9	1180.9	1211.9	1215.5	
C-O	-0.3	-2.5	2.2	1.4	-4.3	-6.1	-0.1	-7.1	-3.5	
OBS.	1027.0	1039.0	1039.0	1081.0	1097.0	1121.0	1181.0	1219.0	1219.0	
IRINT.	3.487	2.748	0.432	3.466	7.679	9.473	1.140	3.579	11.194	
RACT.	3.587	8.981	0.431	2.763	5.024	2.480	1.701	9.785	0.928	
DEPOL.	0.746	0.743	0.638	0.206	0.702	0.681	0.585	0.711	0.666	
NR.	36	35	34	33	32	31	30	29	28	
CALC.	1254.1	1280.9	1288.0	1306.6	1319.9	1345.0	1359.5	1363.8	1380.7	
C-O	-0.9	-1.1	0.0	6.6	8.9	8.0	0.5	4.8	2.7	
OBS.	1255.0	1282.0	1288.0	1300.0	1311.0	1337.0	1359.0	1359.0	1378.0	
IRINT.	4.143	3.686	1.395	0.369	7.230	2.523	0.530	2.016	1.240	
RACT.	3.235	0.694	10.720	6.410	7.319	4.273	5.729	3.700	4.115	
DEPOL.	0.540	0.479	0.537	0.736	0.446	0.637	0.397	0.749	0.616	
NR.	27	26	25	24	23	22	21	20	19	
CALC.	1382.4	1411.5	1427.6	1430.8	1432.9	1436.3	1444.9	1450.8	1451.9	
C-O	4.4	-13.5	2.6	-3.2	-1.1	2.3	-6.1	-0.2	0.9	
OBS.	1378.0	1425.0	1425.0	1434.0	1434.0	1434.0	1451.0	1451.0	1451.0	
IRINT.	13.124	0.040	3.086	4.218	3.782	9.027	8.356	12.060	1.722	
RACT.	3.357	23.749	27.175	5.883	3.749	14.936	11.778	6.093	5.066	
DEPOL.	0.741	0.465	0.710	0.589	0.725	0.747	0.749	0.707	0.705	
NR.	18	17	16	15	14	13	12	11	10	
CALC.	1473.9	1645.2	2888.4	2892.4	2905.1	2909.1	2912.3	2919.5	2930.2	
C-O	5.9	-0.8	-1.6	2.4	15.1	-10.9	-7.7	-0.5	-2.8	
OBS.	1468.0	1646.0	2890.0	2890.0	2890.0	2920.0	2920.0	2920.0	2933.0	
IRINT.	6.374	19.386	9.984	34.010	12.340	37.540	25.857	15.582	36.539	
RACT.	4.374	25.437	38.575	87.416	428.932	165.198	125.961	122.123	115.850	
DEPOL.	0.318	0.157	0.550	0.166	0.496	0.029	0.216	0.107	0.280	
NR.	9	8	7	6	5	4	3	2	1	
CALC.	2951.1	2957.3	2966.1	2968.4	2972.5	2993.7	2998.7	3005.5	3091.6	
C-O	-6.9	-0.7	-1.9	0.4	-0.5	5.7	10.7	-12.5	18.6	
OBS.	2958.0	2958.0	2968.0	2968.0	2973.0	2988.0	2988.0	3018.0	3073.0	
IRINT.	12.142	27.573	35.274	31.047	29.739	22.722	19.945	10.761	20.259	
RACT.	64.309	749.009	103.073	121.201	85.390	160.603	77.621	145.817	91.562	
DEPOL.	0.632	0.749	0.359	0.369	0.748	0.740	0.685	0.137	0.716	

S-(-)-Limonene Oxide, eq-t255 (1.9 kJ/mol)

NR.	75	74	73							
CALC.	42.9	67.3	171.6							
C-O	0.0	0.0	0.0							
OBS.	0.0	0.0	0.0							
IRINT.	0.116	0.581	0.434							
RACT.	2.852	0.375	1.037							
DEPOL.	0.749	0.750	0.722							
NR.	72	71	70	69	68	67	66	65	64	
CALC.	178.7	185.8	208.8	240.0	285.2	315.7	333.4	390.5	429.4	
C-O	-1.3	5.8	0.8	-5.0	-2.8	-6.3	-4.6	-2.5	0.0	
OBS.	180.0	180.0	208.0	245.0	288.0	322.0	338.0	393.0	0.0	
IRINT.	0.498	0.151	1.107	0.922	0.138	1.916	0.586	5.034	3.358	

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RACT.	0.058	0.565	0.629	0.767	2.639	0.472	1.836	1.032	0.711
DEPOL.	0.724	0.739	0.725	0.438	0.298	0.293	0.748	0.344	0.695
NR.	63	62	61	60	59	58	57	56	55
CALC.	457.2	490.3	541.0	553.9	610.1	673.3	694.5	759.7	805.9
C-O	-1.8	2.3	4.0	-3.1	-0.9	-4.7	-6.5	-0.3	-1.1
OBS.	459.0	488.0	537.0	557.0	611.0	678.0	701.0	760.0	807.0
IRINT.	3.908	1.464	1.692	6.842	0.551	5.977	0.514	7.424	4.722
RACT.	0.894	1.651	4.155	1.659	1.720	10.755	5.981	12.754	0.874
DEPOL.	0.750	0.422	0.260	0.730	0.744	0.168	0.380	0.283	0.231
NR.	54	53	52	51	50	49	48	47	46
CALC.	846.0	885.8	897.4	907.2	912.4	967.4	983.0	989.9	1008.1
C-O	3.0	-1.2	-2.6	2.2	-3.6	-2.6	0.0	-8.1	-5.9
OBS.	843.0	887.0	900.0	905.0	916.0	970.0	983.0	998.0	1014.0
IRINT.	15.088	3.242	3.460	27.796	4.252	2.921	1.374	3.852	5.412
RACT.	2.843	1.804	5.033	0.773	1.560	1.145	2.165	4.508	0.793
DEPOL.	0.479	0.691	0.385	0.308	0.116	0.750	0.471	0.722	0.663
NR.	45	44	43	42	41	40	39	38	37
CALC.	1022.3	1039.0	1039.7	1084.5	1098.1	1121.0	1179.9	1202.6	1215.4
C-O	-1.7	0.0	0.7	3.5	1.1	0.0	-1.1	-6.4	-3.6
OBS.	1024.0	1039.0	1039.0	1081.0	1097.0	1121.0	1181.0	1209.0	1219.0
IRINT.	3.871	1.233	1.893	1.696	10.697	4.237	1.125	7.660	13.411
RACT.	3.300	8.343	0.802	2.814	3.179	2.408	1.345	6.161	5.471
DEPOL.	0.283	0.726	0.733	0.108	0.641	0.748	0.613	0.627	0.697
NR.	36	35	34	33	32	31	30	29	28
CALC.	1246.5	1259.7	1298.3	1313.6	1323.2	1336.2	1362.0	1377.7	1381.6
C-O	2.5	4.7	-0.7	2.6	0.0	-0.8	3.0	-0.3	3.6
OBS.	1244.0	1255.0	1299.0	1311.0	0.0	1337.0	1359.0	1378.0	1378.0
IRINT.	2.435	4.913	1.150	2.737	4.196	2.716	1.900	3.306	5.331
RACT.	2.445	2.275	9.589	5.027	5.863	4.292	2.643	5.130	1.496
DEPOL.	0.472	0.736	0.748	0.465	0.719	0.447	0.225	0.650	0.699
NR.	27	26	25	24	23	22	21	20	19
CALC.	1382.1	1409.1	1428.3	1432.0	1434.6	1436.5	1445.1	1449.8	1454.1
C-O	4.1	0.0	3.3	-2.0	0.6	2.5	-5.9	-1.2	3.1
OBS.	1378.0	0.0	1425.0	1434.0	1434.0	1434.0	1451.0	1451.0	1451.0
IRINT.	3.309	0.232	3.310	7.218	6.677	2.391	7.250	15.881	0.249
RACT.	6.308	33.205	25.395	5.277	2.066	7.078	12.968	4.759	4.765
DEPOL.	0.663	0.541	0.673	0.725	0.626	0.748	0.750	0.699	0.699
NR.	18	17	16	15	14	13	12	11	10
CALC.	1474.9	1647.6	2850.4	2891.8	2896.7	2908.2	2909.1	2921.4	2932.5
C-O	6.9	1.6	8.4	1.8	6.7	-11.8	-10.9	1.4	-0.5
OBS.	1468.0	1646.0	2842.0	2890.0	2890.0	2920.0	2920.0	2920.0	2933.0
IRINT.	4.728	20.430	22.906	29.324	23.893	31.634	28.017	11.055	34.819
RACT.	4.038	19.577	62.683	52.587	143.044	50.074	213.275	72.792	100.305
DEPOL.	0.324	0.111	0.270	0.203	0.018	0.198	0.027	0.380	0.190
NR.	9	8	7	6	5	4	3	2	1
CALC.	2945.8	2952.5	2966.7	2970.1	2972.5	2992.1	2998.6	3019.2	3106.5
C-O	-12.2	-5.5	-1.3	2.1	-0.5	4.1	10.6	1.2	24.5
OBS.	2958.0	2958.0	2968.0	2968.0	2973.0	2988.0	2988.0	3018.0	3082.0
IRINT.	26.830	8.988	58.917	12.498	31.726	23.303	20.162	9.271	16.188
RACT.	61.470	48.107	119.689	97.790	80.612	76.970	77.125	149.494	66.198
DEPOL.	0.717	0.716	0.199	0.440	0.732	0.680	0.687	0.157	0.750

S(-)-Limonene Oxide, eq-cl10 (2.0 kJ/mol)

NR.	75	74	73						
CALC.	44.1	78.0	151.4						
C-O	0.0	0.0	0.0						
OBS.	0.0	0.0	0.0						
IRINT.	0.020	0.857	0.497						
RACT.	4.783	0.343	1.066						
DEPOL.	0.715	0.660	0.520						
NR.	72	71	70	69	68	67	66	65	64
CALC.	175.6	182.8	203.8	241.1	262.5	321.3	333.9	401.0	410.6
C-O	-4.4	2.8	-4.2	-3.9	-7.5	-0.7	-4.1	-1.0	0.0
OBS.	180.0	180.0	208.0	245.0	270.0	322.0	338.0	402.0	0.0
IRINT.	0.169	0.436	0.371	0.549	0.972	0.481	0.556	8.206	3.641
RACT.	1.535	0.292	1.250	1.243	1.395	1.676	2.961	0.992	0.580
DEPOL.	0.691	0.720	0.495	0.459	0.198	0.589	0.461	0.733	0.749
NR.	63	62	61	60	59	58	57	56	55
CALC.	467.7	501.1	531.5	558.4	631.0	677.4	708.9	759.0	787.5
C-O	-1.3	-3.9	-1.5	1.4	-2.0	-0.6	7.9	-1.0	-4.5
OBS.	469.0	505.0	533.0	557.0	633.0	678.0	701.0	760.0	792.0
IRINT.	2.168	2.640	4.962	5.136	0.297	4.899	0.543	12.312	1.784
RACT.	1.001	3.719	2.868	1.894	1.306	12.482	3.248	8.966	7.423
DEPOL.	0.523	0.245	0.749	0.704	0.746	0.167	0.621	0.348	0.171
NR.	54	53	52	51	50	49	48	47	46
CALC.	845.5	872.1	899.9	909.6	920.8	948.5	977.0	1006.2	1011.0
C-O	2.5	0.0	-0.1	-6.4	4.8	-1.5	-6.0	8.2	-3.0
OBS.	843.0	0.0	900.0	916.0	916.0	950.0	983.0	998.0	1014.0
IRINT.	12.005	2.555	4.798	30.440	0.538	7.404	1.702	1.023	4.412
RACT.	3.999	1.821	2.838	0.692	2.608	1.794	0.993	6.346	4.681
DEPOL.	0.296	0.696	0.336	0.572	0.604	0.533	0.743	0.154	0.716
NR.	45	44	43	42	41	40	39	38	37
CALC.	1035.7	1040.6	1045.2	1058.5	1097.5	1117.4	1180.7	1196.0	1232.0
C-O	-3.3	1.6	6.2	2.5	0.5	-3.6	-0.3	-1.0	3.0
OBS.	1039.0	1039.0	1039.0	1056.0	1097.0	1121.0	1181.0	1197.0	1229.0
IRINT.	5.341	2.516	4.756	5.653	0.312	14.092	9.939	3.739	6.345
RACT.	1.708	2.943	6.013	5.806	3.315	2.391	2.046	2.821	0.893
DEPOL.	0.654	0.728	0.748	0.750	0.736	0.527	0.498	0.626	0.459
NR.	36	35	34	33	32	31	30	29	28
CALC.	1255.3	1276.0	1284.2	1304.4	1313.6	1349.6	1355.3	1366.4	1380.3

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C-O	0.3	-6.0	-3.8	5.4	2.6	-9.4	-3.7	7.4	2.3
OBS.	1255.0	1282.0	1288.0	1299.0	1311.0	1359.0	1359.0	1378.0	1378.0
IRINT.	4.605	4.879	1.474	1.303	5.115	2.368	0.249	1.976	4.068
RACT.	9.064	2.935	7.114	7.554	8.858	7.853	5.198	6.407	2.142
DEPOL.	0.590	0.567	0.512	0.749	0.472	0.383	0.719	0.748	0.510

NR.	27	26	25	24	23	22	21	20	19
CALC.	1382.1	1411.8	1428.0	1433.3	1435.7	1436.9	1446.2	1451.3	1456.1
C-O	4.1	-13.2	3.0	-0.7	1.7	2.9	-4.8	0.3	5.1
OBS.	1378.0	1425.0	1425.0	1434.0	1434.0	1434.0	1451.0	1451.0	1451.0
IRINT.	10.224	0.238	3.038	5.086	2.526	4.859	6.424	9.859	2.726
RACT.	6.652	23.627	19.896	19.331	2.080	5.874	14.362	3.746	6.901
DEPOL.	0.732	0.442	0.695	0.738	0.680	0.746	0.750	0.641	0.741

NR.	18	17	16	15	14	13	12	11	10
CALC.	1473.2	1645.3	2894.8	2898.1	2904.2	2905.3	2908.7	2925.5	2939.8
C-O	5.2	-0.7	4.8	8.1	-15.8	-14.7	-11.3	5.5	6.8
OBS.	1468.0	1646.0	2890.0	2890.0	2920.0	2920.0	2920.0	2920.0	2933.0
IRINT.	7.457	19.817	11.802	15.476	13.828	31.036	42.081	3.816	49.138
RACT.	1.934	24.996	29.475	43.069	34.559	150.011	274.187	49.332	17.836
DEPOL.	0.138	0.150	0.420	0.743	0.064	0.062	0.039	0.745	0.652

NR.	9	8	7	6	5	4	3	2	1
CALC.	2943.7	2952.9	2954.5	2956.5	2970.4	2992.5	2998.1	3006.5	3093.4
C-O	10.7	-5.1	-3.5	-1.5	-2.6	4.5	10.1	-11.5	20.4
OBS.	2933.0	2958.0	2958.0	2958.0	2973.0	2988.0	2988.0	3018.0	3073.0
IRINT.	7.537	40.947	12.451	57.102	24.504	23.040	20.025	10.495	19.165
RACT.	125.521	42.917	94.575	145.758	83.966	72.796	78.415	146.533	89.881
DEPOL.	0.332	0.353	0.748	0.181	0.750	0.693	0.702	0.132	0.727

S-(-)-Limonene Oxide, eq-c255 (2.5 kJ/mol)

NR.	75	74	73
CALC.	43.7	79.3	152.2
C-O	0.0	0.0	0.0
OBS.	0.0	0.0	0.0
IRINT.	0.638	1.345	0.363
RACT.	3.176	0.538	0.218
DEPOL.	0.749	0.739	0.750

NR.	72	71	70	69	68	67	66	65	64
CALC.	179.0	188.3	204.1	244.5	281.9	317.5	340.4	403.3	417.3
C-O	-1.0	8.3	-3.9	-0.5	-6.1	-4.5	2.4	1.3	0.0
OBS.	180.0	180.0	208.0	245.0	288.0	322.0	338.0	402.0	0.0
IRINT.	0.385	0.098	0.271	0.491	0.512	0.191	1.520	6.691	6.128
RACT.	0.501	0.643	0.580	0.667	3.616	0.748	0.920	0.571	0.981
DEPOL.	0.705	0.748	0.658	0.707	0.282	0.734	0.748	0.614	0.559

NR.	63	62	61	60	59	58	57	56	55
CALC.	443.3	495.1	540.7	551.9	632.1	679.4	693.8	760.7	799.1
C-O	-1.7	7.1	3.7	-5.1	-0.9	1.4	-7.2	0.7	2.1
OBS.	445.0	488.0	537.0	557.0	633.0	678.0	701.0	760.0	797.0
IRINT.	0.330	1.145	4.484	7.201	0.379	5.454	0.279	13.484	2.183
RACT.	0.819	2.426	3.317	1.561	1.492	12.238	7.049	7.048	1.848
DEPOL.	0.614	0.379	0.319	0.556	0.697	0.189	0.342	0.403	0.193

NR.	54	53	52	51	50	49	48	47	46
CALC.	848.4	881.1	901.8	906.6	920.8	950.1	974.7	992.5	1018.7
C-O	5.4	-5.9	1.8	1.6	4.8	0.1	4.7	-5.5	-4.3
OBS.	843.0	887.0	900.0	905.0	916.0	950.0	970.0	998.0	1023.0
IRINT.	11.076	0.970	15.208	19.639	1.148	4.959	3.693	0.393	3.771
RACT.	5.771	1.895	2.175	1.736	1.618	1.067	2.387	1.905	3.406
DEPOL.	0.210	0.381	0.230	0.139	0.743	0.715	0.453	0.746	0.381

NR.	45	44	43	42	41	40	39	38	37
CALC.	1032.9	1036.8	1050.5	1057.3	1106.3	1117.9	1178.5	1193.3	1222.0
C-O	5.9	-2.2	-5.5	1.3	0.0	-3.1	-2.5	-3.7	3.0
OBS.	1027.0	1039.0	1056.0	1056.0	0.0	1121.0	1181.0	1197.0	1219.0
IRINT.	1.439	6.608	3.485	3.973	0.569	12.753	6.424	0.383	13.849
RACT.	1.350	2.408	9.099	5.576	1.883	2.595	2.590	2.606	2.250
DEPOL.	0.484	0.670	0.731	0.693	0.743	0.375	0.215	0.397	0.730

NR.	36	35	34	33	32	31	30	29	28
CALC.	1253.2	1258.4	1288.3	1306.1	1320.9	1342.1	1357.7	1378.1	1381.2
C-O	-1.8	3.4	0.3	-4.9	9.9	5.1	-1.3	0.1	3.2
OBS.	1255.0	1255.0	1288.0	1311.0	1311.0	1337.0	1359.0	1378.0	1378.0
IRINT.	5.032	2.379	4.789	4.866	0.580	1.443	1.925	3.224	6.469
RACT.	4.517	3.650	6.613	10.647	4.769	3.335	2.269	5.414	4.144
DEPOL.	0.658	0.603	0.719	0.549	0.742	0.375	0.458	0.632	0.669

NR.	27	26	25	24	23	22	21	20	19
CALC.	1386.4	1409.2	1428.2	1433.1	1435.2	1436.0	1446.2	1450.5	1458.3
C-O	-8.6	-15.8	3.2	-0.9	1.2	2.0	-4.8	-0.5	7.3
OBS.	1395.0	1425.0	1425.0	1434.0	1434.0	1434.0	1451.0	1451.0	1451.0
IRINT.	2.331	0.301	4.086	0.641	6.558	3.354	6.349	15.822	1.260
RACT.	5.291	33.396	14.815	5.532	14.687	5.634	13.596	5.750	4.556
DEPOL.	0.520	0.567	0.632	0.749	0.750	0.742	0.750	0.689	0.732

NR.	18	17	16	15	14	13	12	11	10
CALC.	1474.7	1647.3	2889.4	2896.4	2899.9	2903.4	2904.2	2908.7	2941.5
C-O	6.7	1.3	-0.6	6.4	9.9	-16.6	-15.8	-11.3	8.5
OBS.	1468.0	1646.0	2890.0	2890.0	2890.0	2920.0	2920.0	2920.0	2933.0
IRINT.	9.785	21.266	1.665	2.883	30.873	40.516	4.841	42.178	30.302
RACT.	1.746	19.433	87.346	30.231	176.675	21.376	16.172	241.932	56.705
DEPOL.	0.121	0.116	0.256	0.231	0.033	0.072	0.688	0.037	0.586

NR.	9	8	7	6	5	4	3	2	1
CALC.	2945.3	2950.7	2955.9	2956.6	2970.7	2992.6	2998.2	3018.6	3103.9
C-O	-12.7	-7.3	-2.1	-1.4	2.7	4.6	10.2	0.6	21.9
OBS.	2958.0	2958.0	2958.0	2958.0	2968.0	2988.0	2988.0	3018.0	3082.0
IRINT.	25.987	16.826	33.933	55.230	24.095	23.800	19.847	9.204	17.170
RACT.	81.484	82.978	73.477	167.635	83.195	75.190	77.648	145.559	67.468
DEPOL.	0.398	0.728	0.442	0.170	0.750	0.687	0.700	0.153	0.748

Supplementary Material (ESI) for *PCCP*  
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S-(-)-Limonene Oxide, eq-c305 (2.8 kJ/mol)

NR.	75	74	73						
CALC.	33.0	76.7	143.8						
C-O	0.0	0.0	0.0						
OBS.	0.0	0.0	0.0						
IRINT.	0.744	4.535	0.385						
RACT.	3.208	0.420	0.159						
DEPOL.	0.749	0.734	0.745						
NR.	72	71	70	69	68	67	66	65	64
CALC.	169.0	185.9	207.8	241.6	288.3	320.7	331.5	396.4	409.1
C-O	-11.0	5.9	-0.2	-3.4	0.3	-1.3	-6.5	3.4	7.1
OBS.	180.0	180.0	208.0	245.0	288.0	322.0	338.0	393.0	402.0
IRINT.	0.601	0.754	1.180	0.738	0.736	0.791	0.814	9.131	4.751
RACT.	0.377	0.913	0.276	0.217	3.855	0.302	1.438	1.076	0.305
DEPOL.	0.732	0.742	0.655	0.342	0.272	0.746	0.744	0.749	0.750
NR.	63	62	61	60	59	58	57	56	55
CALC.	450.8	499.1	522.9	565.4	631.4	674.7	682.4	759.4	791.4
C-O	5.8	-5.9	-3.1	8.4	-1.6	-3.3	4.4	-0.6	-0.6
OBS.	445.0	505.0	526.0	557.0	633.0	678.0	678.0	760.0	792.0
IRINT.	0.137	4.056	7.376	4.818	1.069	8.418	20.170	14.443	0.333
RACT.	1.266	2.078	3.426	1.632	1.603	11.919	4.438	8.685	3.953
DEPOL.	0.703	0.510	0.379	0.335	0.645	0.134	0.594	0.397	0.249
NR.	54	53	52	51	50	49	48	47	46
CALC.	850.3	885.2	903.6	905.3	919.8	947.2	983.0	996.0	1014.8
C-O	7.3	-1.8	-1.4	0.3	3.8	-2.8	0.0	-2.0	0.8
OBS.	843.0	887.0	905.0	905.0	916.0	950.0	983.0	998.0	1014.0
IRINT.	12.254	2.300	27.335	6.386	2.397	3.475	6.081	4.734	3.039
RACT.	4.077	2.143	1.434	2.284	1.586	2.056	1.145	5.367	2.145
DEPOL.	0.144	0.298	0.197	0.260	0.684	0.712	0.161	0.542	0.497
NR.	45	44	43	42	41	40	39	38	37
CALC.	1033.0	1045.0	1052.2	1068.7	1101.6	1120.0	1180.6	1197.0	1213.2
C-O	-6.0	6.0	-3.8	-12.3	4.6	-1.0	-0.4	0.0	-5.8
OBS.	1039.0	1039.0	1056.0	1081.0	1097.0	1121.0	1181.0	1197.0	1219.0
IRINT.	5.336	4.558	1.833	3.527	0.274	15.561	5.287	1.643	5.266
RACT.	2.014	4.048	4.620	1.799	3.983	3.110	1.892	5.919	0.474
DEPOL.	0.750	0.703	0.730	0.505	0.747	0.428	0.400	0.399	0.394
NR.	36	35	34	33	32	31	30	29	28
CALC.	1245.9	1265.8	1297.7	1300.3	1319.0	1343.3	1359.6	1377.2	1380.5
C-O	-9.1	10.8	-1.3	1.3	8.0	6.3	0.6	-0.8	2.5
OBS.	1255.0	1255.0	1299.0	1299.0	1311.0	1337.0	1359.0	1378.0	1378.0
IRINT.	7.295	0.617	3.938	0.665	4.295	2.905	1.657	6.491	0.682
RACT.	3.945	6.744	7.888	4.437	4.132	7.072	2.856	3.223	5.311
DEPOL.	0.564	0.728	0.566	0.746	0.526	0.749	0.358	0.600	0.622
NR.	27	26	25	24	23	22	21	20	19
CALC.	1386.8	1405.1	1427.8	1432.9	1435.2	1436.5	1444.9	1448.8	1456.5
C-O	-8.2	10.1	2.8	-1.1	1.2	2.5	-6.1	-2.2	5.5
OBS.	1395.0	1395.0	1425.0	1434.0	1434.0	1434.0	1451.0	1451.0	1451.0
IRINT.	2.216	7.022	3.670	0.710	10.844	2.294	4.212	16.144	4.847
RACT.	6.106	28.088	15.774	13.945	4.682	2.964	15.118	6.565	9.162
DEPOL.	0.502	0.548	0.707	0.739	0.723	0.717	0.745	0.729	0.744
NR.	18	17	16	15	14	13	12	11	10
CALC.	1475.0	1650.8	2884.3	2897.5	2901.8	2903.1	2906.8	2908.8	2941.6
C-O	7.0	4.8	-5.7	7.5	11.8	-16.9	-13.2	-11.2	8.6
OBS.	1468.0	1646.0	2890.0	2890.0	2890.0	2920.0	2920.0	2920.0	2933.0
IRINT.	8.770	19.542	16.233	18.065	4.043	16.413	47.799	17.073	26.326
RACT.	2.461	19.001	21.258	66.119	262.724	12.155	112.682	84.309	63.315
DEPOL.	0.162	0.121	0.400	0.157	0.060	0.436	0.049	0.057	0.674
NR.	9	8	7	6	5	4	3	2	1
CALC.	2944.0	2953.2	2956.5	2958.4	2970.6	2991.5	2998.7	3019.2	3104.5
C-O	11.0	-4.8	-1.5	0.4	-2.4	3.5	10.7	1.2	22.5
OBS.	2933.0	2958.0	2958.0	2958.0	2973.0	2988.0	2988.0	3018.0	3082.0
IRINT.	16.352	28.487	43.057	55.069	24.104	29.667	17.241	11.565	4.941
RACT.	88.959	89.890	74.764	162.267	79.956	85.486	69.785	133.903	71.898
DEPOL.	0.331	0.721	0.395	0.165	0.750	0.606	0.742	0.148	0.738

**Table 4S:** Potential energy distribution (PED) coming from the output of the MolVib program for the five most stable equatorial conformers (eq-t110, eq-t255, eq-c110, eq-c255 and eq-c305) of the S(-)-Limonene oxide. Contributions to the PED lower than 5% have been omitted. Also, the definition of the internal coordinates used in this work is done.

Definition of the internal coordinates following reference [21]:

Bond stretchings: sij (bond between atoms “i” and “j”)

Torsions and twistings: tccal (carbonyl torsion), tccm1 and tccm2 (methyl torsions); tcci (isopropyl torsion); tccv (vinyl torsion), tccH16 (epoxy ring deformation-torsion).

Six-ring: td (trigonal deformation); adi(i = 1 and 2, asymmetric deformations); p (puckering); ati(i = 1 and 2, asymmetric torsions).

Methyl of the isopropenyl group: sdmi (symmetric deformation); admi1 and admi2 (asymmetric deformations); rmi1 and rmi2 (rockings).

Methylene sp<sup>2</sup> of the vinyl group: sdvi (i = 1 and 2, symmetric deformations); rvi (i = 1 and 2, rockings); wvi (i = 1 and 2, waggings).

Methine sp<sup>2</sup> of the C=C bond in the ring: rch1 (CH rocking); wch1 (CH wagging).

Methylene sp<sup>2</sup> of the C=C bond in the ring: rch2 (rocking); wch2 (wagging).

Epoxy ring: n1, n2 and n3 (epoxy ring deformations).

Methylenes sp<sup>3</sup> of the CH<sub>2</sub> in the ring: tjmeti (i = 1, 2 and 3, CH<sub>2</sub> scissoring); rmeti (i = 1, 2 and 3, CH<sub>2</sub> rocking); wmeti (i = 1, 2 and 3, CH<sub>2</sub> wagging); twmeti (i = 1, 2 and 3, CH<sub>2</sub> twisting).

Methine sp<sup>3</sup> of the chiral carbon: rchqi (i = 1 and 2, CH rocking); dfixcz and dfycz (XCZ and YCZ deformations).



## Supplementary Material (ESI) for PCCP

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Molecule 1 \*oxido de limoneno eq-t110 pred\*

Freq. Main % contributions to the P.E.D. in sym. coordinates

54.	tcci	( 61),	dcq1	( 10),	tccm1	( 10),	at1	( 6)
65.	at1	( 55),	at2	( 23),	p	( 6)		
165.	tccH16	( 26),	dcq1	( 14),	wv2	( 11),	dcq2	( 11), tccm2 ( 9), n2 ( 7)
177.	tccm1	( 37),	tccH16	( 18),	tccm2	( 13),	n1	( 12), wv2 ( 6)
186.	tccm2	( 34),	tccH16	( 22),	tccm1	( 20),	n1	( 11)
208.	at2	( 54),	dcq2	( 11),	dcq1	( 6)		
233.	tccH16	( 48),	n1	( 15),	at2	( 7),	p	( 6), tccm2 ( 6)
281.	ad1	( 20),	tccH16	( 15),	p	( 15),	s47	( 7), sdv2 ( 6), rv2 ( 6)
316.	n1	( 45),	n2	( 14),	tccH16	( 7),	at1	( 7), p ( 6)
318.	n2	( 22),	n3	( 17),	p	( 11),	ad1	( 8), ad2 ( 7), sdv2 ( 7)
387.	tccH16	( 57),	n2	( 11),	p	( 10),	at1	( 7)
440.	n1	( 44),	p	( 15),	n3	( 11),	rv2	( 8)
470.	rv2	( 30),	ad1	( 21),	n1	( 12),	tccH16	( 9), ad2 ( 5)
506.	sdv2	( 20),	tccH16	( 18),	n1	( 16),	dcq2	( 11)
528.	tccH16	( 26),	wv2	( 25),	ad2	( 13),	dcq1	( 9), rmi2 ( 7), n3 ( 5)
560.	tccH16	( 48),	ad2	( 11),	wv2	( 7)		
610.	td	( 25),	s110	( 10),	s47	( 9),	ad2	( 7), s12 ( 6), n4 ( 6)
671.	rO1	( 19),	rO2	( 18),	tccH16	( 13),	s61	( 13), n4 ( 7)
707.	tccv	( 78),	s34	( 6)				
752.	tccH16	( 31),	n4	( 13),	rO1	( 11),	s12	( 6)
794.	tccH16	( 24),	rmet3	( 10),	rmet2	( 9),	n3	( 7), rO1 ( 7), s79 ( 6)
843.	rO2	( 16),	rO1	( 15),	rmet1	( 15),	n3	( 12), tccH16 ( 7), s12 ( 6)
881.	s79	( 28),	rO2	( 17)				
888.	n3	( 21),	rmet2	( 14),	tccH16	( 13),	s34	( 10), rmet1 ( 8), s45 ( 5)
905.	wv	( 77)						
912.	tccH16	( 23),	n3	( 21),	rma2	( 10),	wv	( 6), s61 ( 6), s56 ( 6)
971.	tccH16	( 15),	rma1	( 13),	rO2	( 9),	rmet3	( 9), n4 ( 8)
976.	rv	( 30),	tccH16	( 22),	n3	( 13),	rmi1	( 11)
997.	n3	( 41),	tccH16	( 41)				
1011.	rmi1	( 22),	s23	( 13),	s56	( 10),	s47	( 9), td ( 9)
1027.	tccH16	( 31),	n3	( 12),	rmi1	( 9),	rma1	( 7), twmet3 ( 5)
1036.	n3	( 45),	tccH16	( 44)				
1041.	rmi2	( 39),	tccH16	( 22),	n3	( 22)		
1082.	rmet2	( 13),	p	( 12),	twmet1	( 8),	rmet1	( 7), td ( 6), rmet3 ( 5)
1093.	tccH16	( 57),	n3	( 28)				
1115.	s45	( 18),	s34	( 15),	s23	( 12),	tccH16	( 11)
1181.	tccH16	( 40),	n3	( 23),	twmet2	( 9)		
1212.	tccH16	( 44),	n4	( 22),	n3	( 9),	twmet3	( 9)
1216.	tccH16	( 29),	n4	( 21),	n3	( 14),	twmet1	( 8), s110 ( 6)
1254.	n3	( 29),	tccH16	( 26),	twmet2	( 12),	twmet1	( 6), wmet1 ( 6)
1281.	s47	( 24),	rv	( 18),	s79	( 16),	rv2	( 14)
1288.	rchq2	( 38),	rchq1	( 11),	twmet1	( 11),	twmet3	( 8), wmet1 ( 6)
1307.	n4	( 34),	n3	( 10),	wmet2	( 10),	wmet1	( 10), twmet3 ( 7), rchq1 ( 7)
1320.	n4	( 61),	n3	( 30)				
1345.	rchq1	( 26),	n4	( 15),	wmet1	( 14),	n3	( 13), s34 ( 8), twmet2 ( 5)
1360.	wmet3	( 21),	s61	( 10),	s56	( 9),	wmet2	( 9), wmet1 ( 8), twmet2 ( 7)
1364.	wmet2	( 21),	wmet3	( 18),	n3	( 16),	s61	( 9)
1381.	sdmi	( 47),	sdma	( 26),	n4	( 6),	s79	( 5)
1382.	sdma	( 43),	sdmi	( 19),	n4	( 13),	s110	( 6)
1411.	sdv	( 42),	admi2	( 16),	rchq2	( 8),	admi1	( 8)
1428.	n4	( 36),	n3	( 34),	tjmet1	( 7),	tjmet3	( 6)
1431.	tjmet1	( 31),	n3	( 21),	n4	( 15),	adma1	( 10), adma2 ( 10)
1433.	tjmet3	( 29),	admi1	( 13),	n3	( 11),	adma1	( 11), n4 ( 9), adma2 ( 6)
1436.	admi1	( 42),	tjmet3	( 20),	admi2	( 19),	rmi2	( 5)
1445.	adma2	( 35),	n3	( 22),	adma1	( 17),	n4	( 17)
1451.	admi2	( 34),	admi1	( 22),	sdv	( 15),	tjmet2	( 11), rmi1 ( 6), tjmet1 ( 5)
1452.	tjmet2	( 57),	admi2	( 15),	tjmet3	( 9),	sdv	( 6), tjmet1 ( 5)
1474.	n4	( 38),	n3	( 38),	s12	( 7)		
1645.	s78	( 65),	sdv	( 15),	sdv2	( 5)		
2888.	s419	( 86),	s623	( 6)				
2892.	s623	( 52),	s622	( 34),	s419	( 9)		
2905.	s915	( 39),	s914	( 37),	s913	( 17)		
2909.	s1025	( 42),	s1024	( 36),	s1026	( 20)		
2912.	s317	( 55),	s318	( 33)				
2920.	s521	( 40),	s520	( 31),	s623	( 14),	s622	( 9)
2930.	s622	( 52),	s623	( 24),	s521	( 21)		
2951.	s318	( 46),	s317	( 30),	s216	( 11),	s915	( 6)
2957.	s914	( 44),	s915	( 42),	s317	( 5)		
2966.	s216	( 39),	s520	( 34),	s521	( 17)		
2968.	s216	( 44),	s520	( 26),	s521	( 14),	s318	( 8)
2973.	s1025	( 49),	s1024	( 46)				
2994.	s913	( 80),	s914	( 10),	s915	( 8)		
2999.	s1026	( 78),	s1024	( 15),	s1025	( 6)		
3005.	s812	( 51),	s811	( 47)				
3092.	s811	( 51),	s812	( 48)				



## Supplementary Material (ESI) for PCCP

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Molecule 1 \*oxido de limoneno eq-cl10 pred\*

Freq. Main % contributions to the P.E.D. in sym. coordinates

44.	tcci	( 64),	tccm1	( 18),	dcq1	( 6),	tccv	( 5)				
78.	at1	( 55),	at2	( 18),	tccH16	( 10),	n1	( 5)				
151.	at2	( 48),	dcq1	( 14),	p	( 9),	wv2	( 6),	tccH16	( 6)		
176.	dcq2	( 23),	tccm1	( 21),	at2	( 15),	wv2	( 15),	p	( 6)		
183.	tccm1	( 57),	tccH16	( 11),	dcq2	( 6)						
204.	tccH16	( 35),	n1	( 26),	tccm2	( 24)						
241.	tccH16	( 45),	tccm2	( 14),	n1	( 10),	at2	( 7),	p	( 6)		
263.	n1	( 18),	sdv2	( 18),	ad1	( 12),	tccH16	( 7),	at1	( 6),	s47	( 6)
321.	n2	( 43),	n1	( 21),	ad2	( 9),	n3	( 6)				
334.	p	( 19),	ad1	( 14),	rv2	( 10),	sdv2	( 8),	n3	( 8),	n1	( 6)
401.	tccH16	( 70),	p	( 9),	at1	( 8)						
411.	n1	( 50),	ad2	( 10),	p	( 6),	at1	( 6),	n3	( 6)		
468.	rv2	( 43),	ad1	( 22),	ad2	( 8),	rv	( 5)				
501.	sdv2	( 20),	n1	( 14),	tccH16	( 14),	dcq2	( 10),	dcq1	( 6),	p	( 6)
532.	wv2	( 35),	dcq1	( 12),	tccH16	( 11),	rmi2	( 10),	ad2	( 7)		
558.	tccH16	( 24),	ad2	( 10),	n1	( 8),	dcq2	( 7),	wv2	( 7),	ad1	( 6)
631.	td	( 24),	s47	( 11),	s110	( 10),	ad2	( 9),	s34	( 7),	s12	( 7)
677.	rO2	( 20),	rO1	( 14),	s61	( 11),	tccH16	( 8),	s12	( 6),	p	( 6)
709.	tccv	( 78),	s34	( 6)								
759.	tccH16	( 41),	rO1	( 16),	n4	( 13)						
787.	rmet3	( 20),	rmet2	( 16),	tccH16	( 14),	s79	( 7),	rmet1	( 6),	n3	( 6)
846.	rO2	( 22),	rmet1	( 13),	rmet2	( 10),	rO1	( 7),	s12	( 6),	n4	( 6)
872.	s79	( 30),	s45	( 9),	n3	( 9),	s34	( 7),	tccH16	( 6)		
900.	n3	( 39),	tccH16	( 25)								
910.	wv	( 91)										
921.	rmet1	( 13),	rma1	( 13),	s23	( 9),	rmet3	( 7),	rma2	( 7),	twmet2	( 6)
949.	n4	( 14),	rO2	( 14),	td	( 7),	n3	( 7),	rmet2	( 6),	s23	( 6)
977.	rv	( 41),	rmi1	( 15),	tccH16	( 12),	n3	( 9)				
1006.	tccH16	( 38),	n3	( 21),	s56	( 9),	rmi1	( 6)				
1011.	tccH16	( 32),	n3	( 30),	rmi1	( 8),	rma1	( 7)				
1036.	tccH16	( 40),	n3	( 14),	rma2	( 12),	rmi2	( 5)				
1041.	rmi2	( 41),	s56	( 9),	rmi1	( 6)						
1045.	n3	( 51),	tccH16	( 39)								
1058.	tccH16	( 43),	n3	( 14),	n4	( 7)						
1098.	tccH16	( 33),	n3	( 21),	s45	( 12),	s34	( 9)				
1117.	tccH16	( 54),	n3	( 15),	n4	( 8)						
1181.	n3	( 20),	twmet1	( 15),	twmet2	( 13),	tccH16	( 12),	rchq1	( 9),	n4	( 6)
1196.	tccH16	( 49),	n3	( 18),	n4	( 16),	twmet3	( 5)				
1232.	tccH16	( 43),	n3	( 25),	n4	( 12)						
1255.	twmet2	( 25),	wmet2	( 12),	wmet1	( 12),	twmet1	( 9),	s56	( 6)		
1276.	n4	( 22),	s47	( 9),	tccH16	( 9),	wmet1	( 7),	twmet1	( 6),	s79	( 6)
1284.	rchq2	( 18),	rv	( 12),	s47	( 12),	rchq1	( 11),	rv2	( 9),	s79	( 9)
1304.	n4	( 42),	n3	( 25),	twmet3	( 8),	wmet2	( 6)				
1314.	n4	( 59),	n3	( 30)								
1350.	rchq1	( 22),	n4	( 15),	n3	( 10),	twmet2	( 9),	rchq2	( 8),	wmet1	( 7)
1355.	wmet3	( 28),	n4	( 16),	wmet1	( 10),	s61	( 9),	tccH16	( 7)		
1366.	wmet2	( 27),	wmet3	( 9),	sdmi	( 8),	sdv	( 7),	rchq2	( 7),	n3	( 7)
1380.	sdmi	( 38),	sdma	( 35),	s110	( 5)						
1382.	sdma	( 35),	sdmi	( 24),	n4	( 13)						
1412.	sdv	( 42),	admi2	( 17),	rchq2	( 9),	adm1	( 6)				
1428.	n4	( 36),	n3	( 33),	tjmet3	( 12),	adma2	( 9)				
1433.	tjmet1	( 37),	adma2	( 20),	tjmet2	( 13),	adm1	( 10)				
1436.	tjmet3	( 23),	tjmet1	( 22),	n3	( 21),	n4	( 20),	adma2	( 9)		
1437.	adm1	( 55),	admi2	( 18),	rmi2	( 6),	tjmet1	( 6),	tjmet3	( 6),	adma2	( 6)
1446.	adma1	( 58),	n3	( 18),	n4	( 14)						
1451.	admi2	( 51),	sdv	( 21),	adm1	( 14),	rmi1	( 7)				
1456.	tjmet2	( 76),	tjmet1	( 9),	tjmet3	( 7)						
1473.	n4	( 41),	n3	( 39),	s12	( 7)						
1645.	s78	( 65),	sdv	( 15),	sdv2	( 5)						
2895.	s520	( 70),	s521	( 15)								
2898.	s317	( 54),	s318	( 24),	s914	( 9),	s915	( 6)				
2904.	s623	( 32),	s622	( 18),	s1025	( 16),	s1026	( 14),	s1024	( 7)		
2905.	s914	( 27),	s915	( 27),	s913	( 12),	s520	( 7),	s317	( 7),	s318	( 6)
2909.	s623	( 32),	s1025	( 23),	s1026	( 19),	s622	( 11),	s1024	( 11)		
2926.	s419	( 69),	s318	( 18),	s521	( 7)						
2940.	s521	( 34),	s318	( 30),	s317	( 17),	s622	( 9)				
2944.	s622	( 37),	s318	( 14),	s419	( 13),	s623	( 12),	s521	( 10),	s317	( 10)
2953.	s521	( 25),	s622	( 17),	s623	( 17),	s520	( 13),	s419	( 9),	s914	( 6)
2954.	s915	( 44),	s914	( 42)								
2956.	s216	( 95)										
2970.	s1025	( 50),	s1026	( 47)								
2992.	s913	( 81),	s914	( 9),	s915	( 9)						
2998.	s1024	( 78),	s1026	( 15),	s1025	( 6)						
3006.	s811	( 50),	s812	( 48)								
3093.	s812	( 51),	s811	( 48)								



## Supplementary Material (ESI) for PCCP

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Molecule 1 \*oxido de limoneno eq-c305 pred\*

Freq. Main % contributions to the P.E.D. in sym. coordinates

33.	tcci	( 49),	tccm1	( 17),	dcq2	( 9),	wv2	( 5)				
77.	at1	( 49),	at2	( 9),	tccH16	( 9),	dcq2	( 7)				
144.	at2	( 47),	dcq1	( 11),	p	( 11),	tccm1	( 10),	tccH16	( 6)		
169.	tccm1	( 26),	at2	( 17),	dcq2	( 17),	tccv	( 7),	at1	( 6),	tccm2	( 6)
186.	tccm1	( 40),	wv2	( 16),	tccm2	( 12),	dcq2	( 11),	dcq1	( 6)		
208.	tccH16	( 36),	n1	( 27),	tccm2	( 21)						
242.	tccH16	( 47),	n1	( 14),	tccm2	( 10),	at2	( 7)				
288.	rv2	( 15),	ad1	( 13),	dcq1	( 13),	at1	( 12),	n1	( 8),	s47	( 8)
321.	n2	( 31),	n1	( 27),	ad2	( 10),	n3	( 9),	tccH16	( 6)		
332.	p	( 26),	sdv2	( 19),	n2	( 13),	ad1	( 11),	at1	( 6),	wv2	( 5)
396.	tccH16	( 70)										
409.	n1	( 46),	p	( 13),	at1	( 9),	ad2	( 8),	n3	( 7)		
451.	ad1	( 25),	sdv2	( 20),	rv2	( 6),	dcq1	( 5)				
499.	rv2	( 33),	dcq1	( 16),	wv2	( 15),	rv	( 5)				
523.	tccH16	( 24),	n1	( 15),	wv2	( 13),	td	( 5),	rv2	( 5)		
565.	tccH16	( 18),	wv2	( 11),	ad2	( 10),	dcq2	( 9),	ad1	( 6),	n1	( 6)
631.	td	( 25),	s47	( 10),	s110	( 10),	ad2	( 9),	s34	( 7),	s12	( 7)
675.	tccv	( 20),	rO2	( 13),	rO1	( 11),	s61	( 8),	s45	( 7)		
682.	tccv	( 43),	rO2	( 10),	tccH16	( 5)						
759.	tccH16	( 42),	rO1	( 16),	n4	( 13),	n1	( 5)				
791.	rmet3	( 20),	rmet2	( 17),	tccH16	( 12),	rmet1	( 10),	n3	( 6),	s45	( 5)
850.	rO2	( 25),	rmet2	( 9),	rmet1	( 7),	rO1	( 6),	s12	( 6),	n4	( 6)
885.	s79	( 22),	tccH16	( 17),	n3	( 14),	s45	( 8),	s34	( 7),	rmet1	( 6)
904.	wv	( 34),	n3	( 24),	tccH16	( 11)						
905.	n3	( 28),	wv	( 23),	tccH16	( 15)						
920.	rmet1	( 14),	rma1	( 14),	s23	( 10),	rma2	( 6),	s56	( 6),	rmet3	( 6)
947.	rO2	( 11),	n4	( 11),	s79	( 8),	rmet2	( 8),	s45	( 7),	td	( 6)
983.	s47	( 16),	rmi1	( 15),	s23	( 10),	td	( 8),	rv	( 7)		
996.	tccH16	( 25),	n3	( 20),	rmi1	( 14),	rv	( 12),	rma1	( 8)		
1015.	tccH16	( 49),	n3	( 27),	s56	( 7)						
1033.	tccH16	( 28),	n3	( 17),	rma2	( 12),	rmi2	( 7)				
1045.	n3	( 52),	tccH16	( 37)								
1052.	tccH16	( 45),	n3	( 21),	rmi2	( 6)						
1069.	rmi2	( 20),	n4	( 9),	p	( 6)						
1102.	tccH16	( 49),	n3	( 21),	s45	( 6)						
1120.	tccH16	( 48),	n3	( 12),	n4	( 8)						
1181.	tccH16	( 26),	n3	( 25),	twmet2	( 13),	twmet1	( 9),	rchq1	( 5)		
1197.	tccH16	( 42),	n4	( 21),	n3	( 12),	twmet3	( 6)				
1213.	tccH16	( 43),	n3	( 25),	n4	( 9)						
1246.	tccH16	( 35),	n3	( 17),	n4	( 14),	twmet3	( 8),	wmet2	( 5)		
1266.	twmet1	( 26),	twmet2	( 17),	tccH16	( 9),	rchq2	( 6)				
1298.	n4	( 46),	n3	( 25),	rchq2	( 6)						
1300.	wmet1	( 23),	twmet3	( 14),	rchq1	( 13),	wmet2	( 10),	twmet1	( 8),	s23	( 5)
1319.	n4	( 60),	n3	( 29)								
1343.	wmet2	( 25),	rchq1	( 15),	rchq2	( 12),	twmet2	( 12),	s56	( 7),	s45	( 7)
1360.	wmet3	( 35),	s61	( 14),	wmet2	( 11),	n3	( 6),	tccH16	( 6)		
1377.	sdmi	( 31),	sdma	( 30),	wmet1	( 8),	rchq1	( 7)				
1381.	sdmi	( 40),	sdma	( 32),	n4	( 7)						
1387.	sdma	( 13),	wmet1	( 13),	rchq1	( 11),	n4	( 11),	s47	( 8),	s34	( 7)
1405.	sdv	( 59),	admi1	( 12),	s78	( 7)						
1428.	n4	( 32),	n3	( 28),	tjmet3	( 22)						
1433.	adma2	( 27),	n3	( 22),	n4	( 19),	admi2	( 10),	tjmet2	( 7)		
1435.	tjmet1	( 49),	admi2	( 32),	n4	( 7)						
1436.	tjmet3	( 22),	n3	( 18),	n4	( 15),	tjmet1	( 11),	admi2	( 11),	adma2	( 8)
1445.	admi1	( 30),	adma1	( 25),	n3	( 13),	n4	( 11)				
1449.	adma1	( 44),	admi1	( 20),	n3	( 8),	sdv	( 7),	n4	( 6)		
1456.	tjmet2	( 67),	tjmet1	( 12),	admi2	( 6)						
1475.	n4	( 42),	n3	( 39),	s12	( 7)						
1651.	s78	( 64),	sdv	( 16)								
2884.	s419	( 43),	s915	( 24),	s914	( 11),	s913	( 10),	s520	( 9)		
2898.	s520	( 50),	s317	( 19),	s318	( 9),	s915	( 6),	s521	( 5)		
2902.	s317	( 38),	s318	( 18),	s914	( 11),	s520	( 9),	s915	( 8),	s419	( 7)
2903.	s623	( 43),	s622	( 22),	s1025	( 11),	s1026	( 10),	s1024	( 5)		
2907.	s419	( 28),	s1025	( 15),	s1026	( 13),	s520	( 11),	s1024	( 8),	s521	( 7)
2909.	s623	( 22),	s1025	( 16),	s419	( 16),	s1026	( 13),	s1024	( 7),	s914	( 7)
2942.	s318	( 61),	s317	( 35)								
2944.	s622	( 58),	s521	( 18),	s623	( 18)						
2953.	s914	( 46),	s915	( 46)								
2956.	s521	( 62),	s520	( 16),	s623	( 10),	s622	( 8)				
2958.	s216	( 94)										
2971.	s1025	( 49),	s1026	( 48)								
2992.	s913	( 79),	s914	( 12),	s915	( 6)						
2999.	s1024	( 78),	s1026	( 15),	s1025	( 6)						
3019.	s811	( 63),	s812	( 36)								
3104.	s812	( 63),	s811	( 36)								