The atmospheric impacts of monoterpene ozonolysis on global stabilised Criegee intermediate budgets and SO_2 oxidation: experiment, theory and modeling

GEOS-Chem Modeling

Table S1. Rate constants (cm^3 s^{-1}) used in GEOS-Chem modeling for reactions of monoterpenes with O_3, OH and NO_3. Rate constants are taken from MCMv3.3.1 (http://mcm.leeds.ac.uk/MCM/ (Jenkin et al., 2015)) for α-pinene, β-pinene and limonene, and from the IUPAC Evaluated kinetic and photochemical data for atmospheric chemistry for the other monoterpenes (http://iupac.pole-ether.fr/ (Atkinson et al., 2006)).

Monoterpene	**10^{15} k(MT+O_3) (cm^3 s^{-1})**	**10^{11} k(MT+OH) (cm^3 s^{-1})**	**10^{11} k(MT+NO_3) (cm^3 s^{-1})**
α-pinene	0.805*exp(-640/T)	1.2*exp(440/T)	0.12*exp(490/T)
β-pinene	1.35*exp(-1270/T)	2.38*exp(357/T)	0.251
limonene	2.80*exp(-770/T)	4.28*exp(401/T)	1.22
myrcene	2.65*exp(-520/T)	0.919*exp(1071/T)	1.10
ocimene	4.0*exp(-625/T)	4.35*exp(579/T)	2.20
sabinene	0.082	11.7	1.00
3-carene	0.048	8.80	0.910

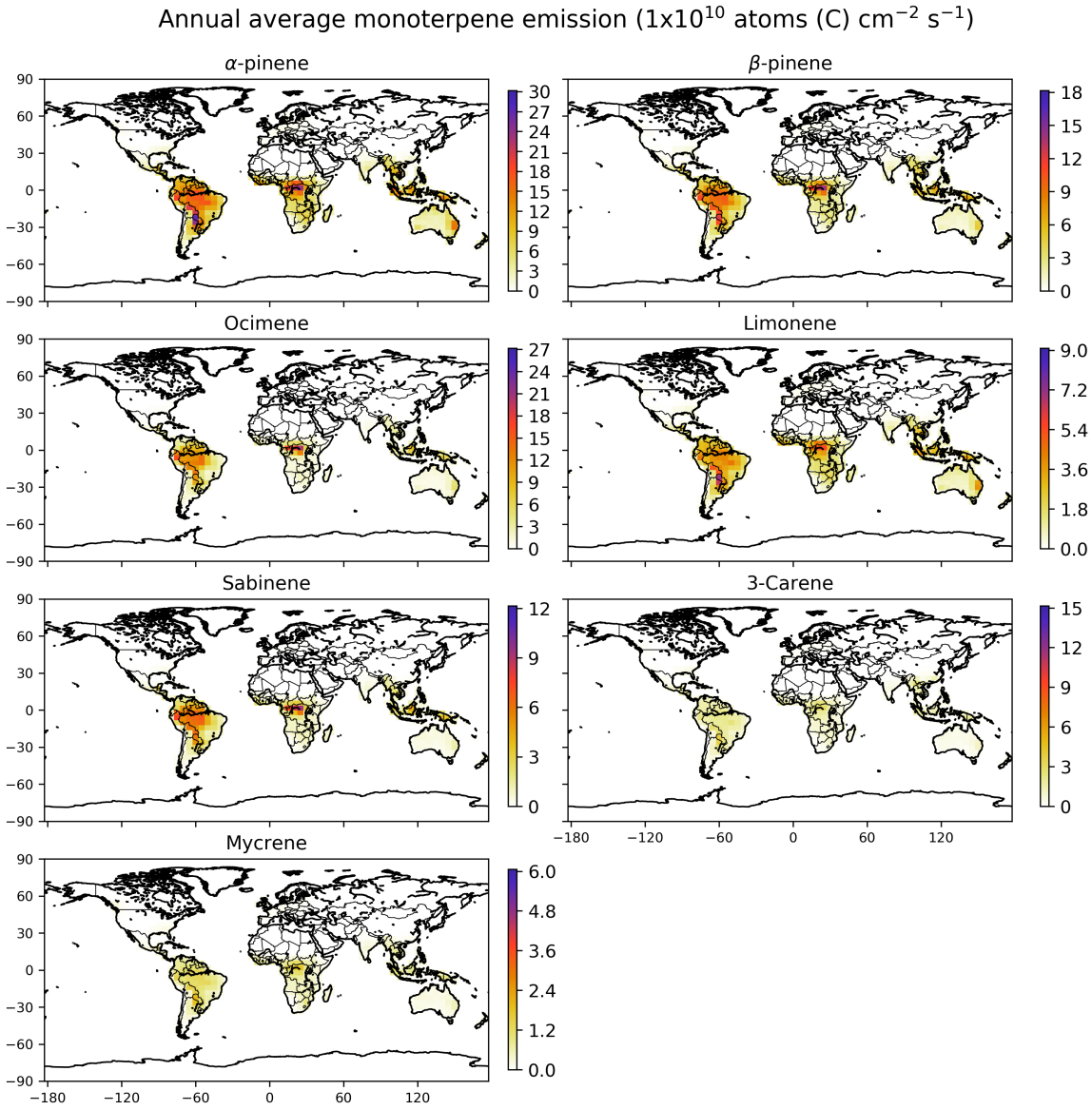


Figure S1. Annual mean monoterpene emission rates (atoms C cm^{-2} s^{-1}) in the GEOS-Chem model simulation, taken from MEGAN v2.1.

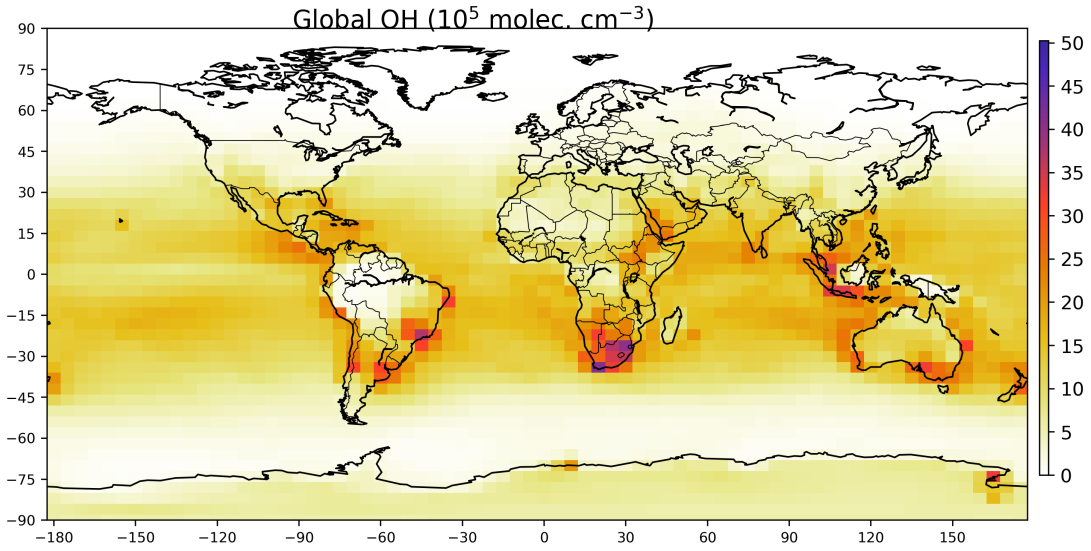


Figure S2. Annual mean OH concentrations (cm^{-3}) in the GEOS-Chem model simulation.

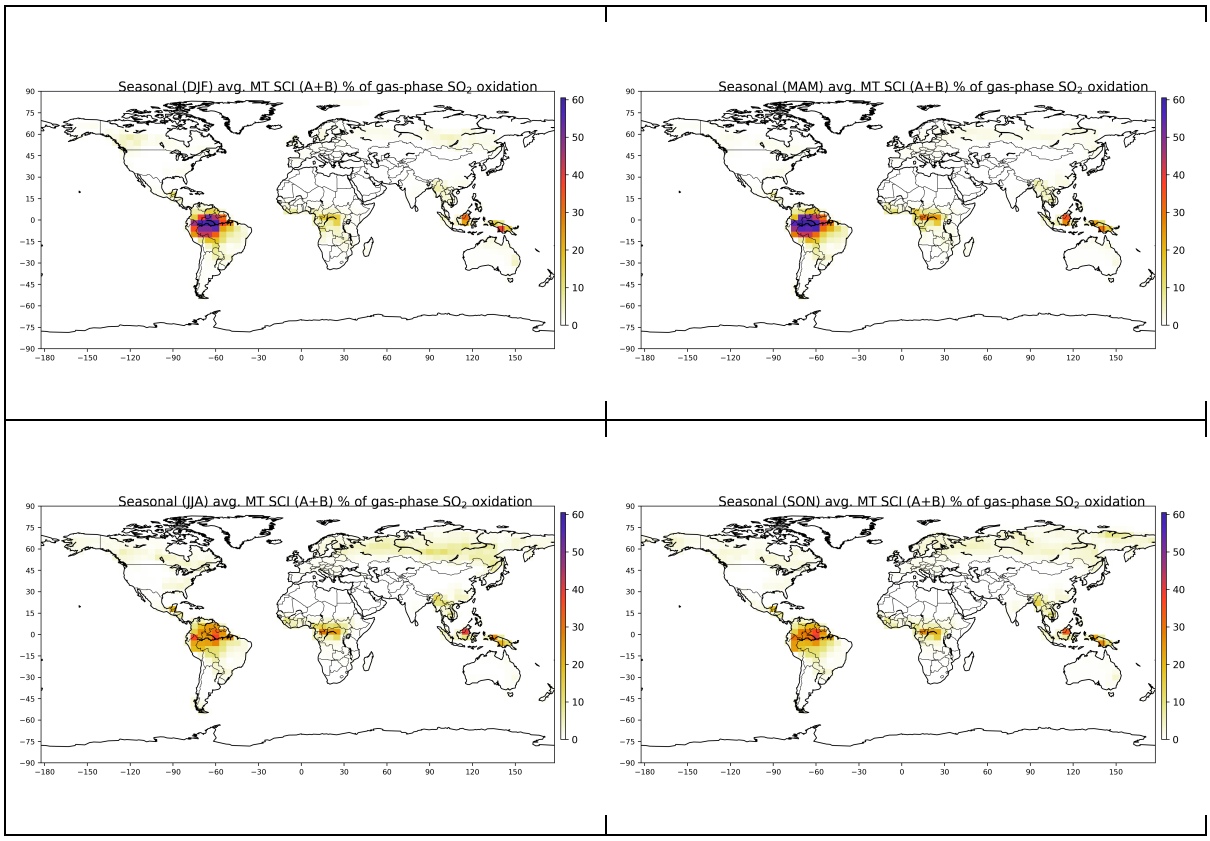
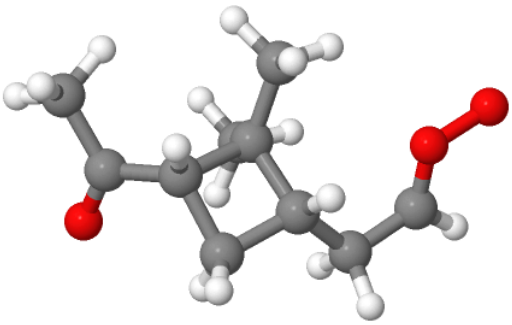
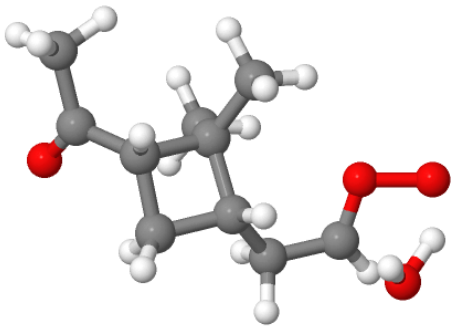


Figure S3. Seasonal SO_2 oxidation by monoterpene derived SCI as percentage of total gas-phase SO_2 oxidation in the surface layer using an alternative $k(SO_2+OH)$ from Blitz et al. (2017).

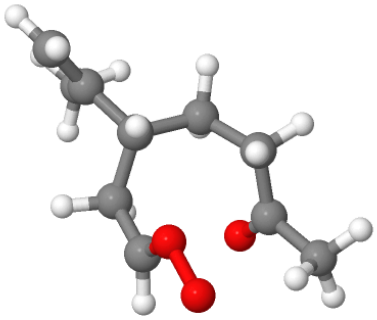
Comparison α-pinene-CI to limonene-CI



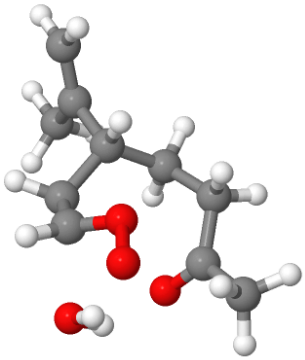
(1) α-pinene-CI-1b



(2) TS : α-pinene-CI-1b + H_2O



(3) Limonene-CI-5b



(4) TS: Limonene-CI-5b + H_2O

Figure S4. Ball and Stick figures of the lowest-energy goemetries anti-RCHOO Criegee intermediates formed from α-pinene and limonene, and their transition states for reaction with a H_2O molecule.

The figure above shows the impact of the four-membered ring on the geometry of the CI, and the transition states for the reaction with water. Panels (1) and (3) show the lowest-energy conformers of the *anti*-RCHOO Criegee intermediates formed from α-pinene and limonene. The 4-membered ring in α-pinene has a most favourable puckering geometry keeping the carbonyl- and carbonyl-oxide bearing substituents in α-pinene-CI-1b on opposite sides. In limonene-CI-5b, these two branches form an intramolecular complex, as also seen in the pre-reactive complex in reactions of CI with ketones and aldehydes. This geometry is suitable to lead to secondary ozonides (SOZ) by cycloaddition.

The transition states for the reaction with an H_2O molecule retains this difference in geometry, shown in panels (2) and (4), where limonene-CI-5b allows the H_2O co-reactant to form

intramolecular H-bonds with the carbonyl bond on the other side of the molecule, lowering the TS energy. Note that reaction through this TS is not necessarily the most dominant channel, as the cyclic structure with H-bonds are entropically less favourable than more elongated structures. Technically such H-bonding is also possible in α-pinene-CI-1b, but this requires additional energy to reverse the puckering of the 4-membered ring, making such a structure unfavourable to the point where it is no longer a saddlepoint on the potential energy surface.

Relative energies (kcal/mol) and partition functions (m^{-3}) of all limonene-CI-5b conformers

Compound	Qtot	Erel
limoneneCI.J.a.pmpctc	2.995e+44	0.00
limoneneCI.J.a.cmpctc	2.394e+44	0.36
limoneneCI.J.a.lmpctc	2.138e+44	0.58
limoneneCI.J.a.cmmctm	4.739e+44	1.74
limoneneCI.J.a.pmmctm	3.779e+44	1.79
limoneneCI.J.a.cmmctc	3.053e+44	2.00
limoneneCI.J.a.mmmctm	4.781e+44	2.54
limoneneCI.J.a.pmmctc	6.330e+44	2.72
limoneneCI.J.a.cmpctm	4.907e+44	2.77
limoneneCI.J.a.ptpcmp	2.375e+45	3.80
limoneneCI.J.a.pttcmp	2.236e+46	5.17
limoneneCI.J.a.lmmctc	4.072e+44	3.10
limoneneCI.J.a.mmpctm	4.054e+44	3.15
limoneneCI.J.a.ptpctm	3.554e+45	4.56
limoneneCI.J.a.pttcmm	2.163e+46	5.65
limoneneCI.J.a.ptpcmm	4.402e+45	4.73
limoneneCI.J.a.ltpcpp	1.165e+46	5.41
limoneneCI.J.a.ptmcmp	8.752e+44	3.92
limoneneCI.J.a.ptmcmm	1.189e+45	4.13
limoneneCI.J.a.mtpctm	1.735e+46	5.73
limoneneCI.J.a.ptmctm	1.699e+45	4.40
limoneneCI.J.a.ptmctc	7.577e+44	4.09
limoneneCI.J.a.ptpcmc	3.580e+45	5.08
limoneneCI.J.a.pttctm	2.760e+46	6.36
limoneneCI.J.a.ptpcpm	1.412e+45	4.60
limoneneCI.J.a.lttcmc	6.518e+45	5.52
limoneneCI.J.a.pmtctm	1.624e+45	4.73
limoneneCI.J.a.mtpcmp	1.940e+45	4.84
limoneneCI.J.a.pttctc	9.494e+45	5.83
limoneneCI.J.a.ptmcmc	7.706e+44	4.38
limoneneCI.J.a.ltpcmc	1.962e+45	4.97
limoneneCI.J.a.pttcmc	8.735e+45	5.86
limoneneCI.J.a.ltpctm	9.187e+45	5.96
limoneneCI.J.a.pmpcpm	9.493e+44	4.63
limoneneCI.J.a.pttcpm	4.642e+45	5.58
limoneneCI.J.a.lpmctc	1.159e+45	4.77
limoneneCI.J.a.cpmptc	1.828e+44	3.69
limoneneCI.J.a.pmpcmm	8.481e+45	6.01
limoneneCI.J.a.cppctm	1.985e+45	5.15
limoneneCI.J.a.cpmcmp	4.026e+45	5.65
limoneneCI.J.a.pttctp	2.498e+46	6.74
limoneneCI.J.a.mmmcpp	5.953e+45	5.89

limoneneCI.J.a.cpmctp 2.216e+45 5.34

limoneneCI.J.a.pmmcmm 2.274e+46 6.74

limoneneCI.J.a.ptpcpp 1.201e+45 4.99

limoneneCI.J.a.pmtcmm 3.166e+46 6.96

limoneneCI.J.a.ltpcmp 5.872e+45 6.00

limoneneCI.J.a.pmmcmp 1.096e+46 6.38

limoneneCI.J.a.ptmctp 1.611e+45 5.25

limoneneCI.J.a.ltpcmm 5.486e+45 5.98

limoneneCI.J.a.ptpctp 4.320e+45 5.87

limoneneCI.J.a.lttcmp 3.866e+45 5.80

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limoneneCI.J.a.ltpcpm 6.862e+45 6.17

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limoneneCI.J.a.lttcpp 2.812e+46 7.02

limoneneCI.J.a.cmmcmm 4.398e+45 5.97

limoneneCI.J.a.pmpcmp 4.461e+45 5.98

limoneneCI.J.a.cptcpp 6.344e+44 4.84

limoneneCI.J.a.cmmcmp 5.018e+45 6.09

limoneneCI.J.a.lttcmm 4.443e+45 6.03

limoneneCI.J.a.mtpcpm 6.751e+45 6.28

limoneneCI.J.a.pptmpc 1.120e+44 3.85

limoneneCI.J.a.lmmcpp 1.000e+46 6.55

limoneneCI.J.a.pmtcmp 1.619e+46 6.84

limoneneCI.J.a.ptmcpm 1.464e+45 5.41

limoneneCI.J.a.cmmcmc 5.224e+45 6.17

limoneneCI.J.a.cptcmp 8.773e+45 6.49

limoneneCI.J.a.cptctm 4.437e+45 6.13

limoneneCI.J.a.pmmptm 1.069e+45 5.29

limoneneCI.J.a.lttcpm 2.464e+46 7.17

limoneneCI.J.a.cppcmp 7.866e+44 5.14

limoneneCI.J.a.ptpctc 1.678e+45 5.62

limoneneCI.J.a.mmpcpm 1.807e+45 5.68

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limoneneCI.J.a.ptpmtm 5.396e+44 5.01

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limoneneCI.J.a.ptpmtc 4.936e+44 4.98

limoneneCI.J.a.cmtctm 1.022e+45 5.44

limoneneCI.J.a.cptcmm 1.579e+46 7.12

limoneneCI.J.a.cppcmm 1.109e+45 5.57

limoneneCI.J.a.pmtctp 7.213e+45 6.70

limoneneCI.J.a.pmtctc 8.921e+45 6.83

limoneneCI.J.a.cttctc 6.891e+45 6.68

limoneneCI.J.a.lmtcmc 1.482e+46 7.14

limoneneCI.J.a.lttctc 6.869e+45 6.68

limoneneCI.J.a.lmpmpc 3.152e+44 4.89

limoneneCI.J.a.cmpcmm 6.640e+45 6.71

limoneneCI.J.a.ptpmmp 4.209e+45 6.45

limoneneCI.J.a.ltpmtc 7.412e+44 5.42

limoneneCI.J.a.mmmptm 1.262e+45 5.74

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limoneneCI.J.a.ltpcpc 4.832e+45 6.56

limoneneCI.J.a.cptcmc 1.191e+46 7.10

limoneneCI.J.a.cppctc 6.465e+44 5.37

limoneneCI.J.a.pmpcmc 4.045e+45 6.48

limoneneCI.J.a.ptpcpc 2.909e+45 6.29

limoneneCI.J.a.pmmpmp 3.869e+45 6.46

limoneneCI.J.a.cmtctc 8.641e+45 7.00

limoneneCI.J.a.cmmptm 1.107e+45 5.78

limoneneCI.J.a.ltpmtm 6.217e+45 6.85

limoneneCI.J.a.lptcmc 7.204e+45 6.94

limoneneCI.J.a.lttctp 1.880e+46 7.52

limoneneCI.J.a.cmmcpp 2.442e+45 6.35

limoneneCI.J.a.ppmcpp 4.724e+43 4.02

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limoneneCI.J.a.mmmcpc 1.989e+46 7.72

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limoneneCI.J.a.ltmptm 1.717e+45 7.56

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limoneneCI.J.a.cppmtm 5.631e+44 7.34

limoneneCI.J.a.ltmpmp 5.410e+44 7.33

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limoneneCI.J.a.pttmmc 4.421e+45 8.61

limoneneCI.J.a.pttppp 4.443e+45 8.61

limoneneCI.J.a.pttmpc 2.913e+46 9.75

limoneneCI.J.a.pptctm 5.222e+45 8.72

limoneneCI.J.a.ltmppm 1.277e+45 7.91

limoneneCI.J.a.lmtcpc 1.024e+46 9.15

limoneneCI.J.a.ptpmpp 1.999e+45 8.20

limoneneCI.J.a.pttmpm 1.855e+45 8.15

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limoneneCI.J.a.lttppp 9.391e+45 9.13

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limoneneCI.J.a.pmpcpc 1.852e+45 8.17

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limoneneCI.J.a.ptmpmp 1.123e+45 7.88

limoneneCI.J.a.lmpmmc 2.003e+45 8.23

limoneneCI.J.a.cptmtc 7.148e+45 8.99

limoneneCI.J.a.ptpmpm 1.678e+45 8.13

limoneneCI.J.a.pmtmtc 2.377e+46 9.71

limoneneCI.J.a.cppcpc 1.325e+44 6.64

limoneneCI.J.a.lpmpmc 1.190e+45 7.96

limoneneCI.J.a.mttptm 1.308e+46 9.40

limoneneCI.J.a.lttmmp 2.264e+45 8.38

limoneneCI.J.a.lptpmc 5.562e+45 8.93

limoneneCI.J.a.cmtcpc 3.976e+45 8.75

limoneneCI.J.a.lttmtm 1.208e+46 9.42

limoneneCI.J.a.cmmppm 1.915e+45 8.33

limoneneCI.J.a.ppmcmm 2.431e+45 8.48

limoneneCI.J.a.cptmmp 8.529e+45 9.23

limoneneCI.J.a.cptcpc 1.390e+45 8.15

limoneneCI.J.a.pttppm 2.757e+45 8.57

limoneneCI.J.a.mttptc 5.906e+45 9.02

limoneneCI.J.a.mttmtm 1.086e+46 9.39

limoneneCI.J.a.lttptm 1.389e+46 9.54

limoneneCI.J.a.lttpmm 9.856e+45 9.34

limoneneCI.J.a.cptpmp 5.345e+45 8.98

limoneneCI.J.a.lttpmc 2.569e+45 8.56

limoneneCI.J.a.mmmpmp 2.094e+45 8.46

limoneneCI.J.a.cppmmc 4.980e+44 7.63

limoneneCI.J.a.pmtppp 6.354e+44 7.78

limoneneCI.J.a.cppmmm 9.535e+44 8.02

limoneneCI.J.a.pttmtp 1.308e+46 9.59

limoneneCI.J.a.cpmpmp 7.595e+45 9.26

limoneneCI.J.a.ctmctc 1.706e+45 8.38

limoneneCI.J.a.lmtmmc 5.513e+45 9.09

limoneneCI.J.a.pttmpp 1.274e+46 9.60

limoneneCI.J.a.cmtppp 5.084e+44 7.68

limoneneCI.J.a.ptpptc 2.425e+45 8.62

limoneneCI.J.a.ltmptp 2.983e+45 8.75

limoneneCI.J.a.cptpmc 5.534e+45 9.13

limoneneCI.J.a.mttmmm 3.045e+45 8.78

limoneneCI.J.a.ptmptm 1.649e+45 8.42

limoneneCI.J.a.lpmpmp 4.651e+45 9.07

limoneneCI.J.a.mptcmp 2.254e+45 8.63

limoneneCI.J.a.pmpcpp 1.379e+45 8.36

limoneneCI.J.a.lpmpmm 3.479e+45 8.91

limoneneCI.J.a.ctmcmp 3.010e+45 8.84

limoneneCI.J.a.lpmcpm 7.950e+44 8.05

limoneneCI.J.a.ctmctm 3.185e+45 8.89

limoneneCI.J.a.pptctc 4.811e+45 9.15

limoneneCI.J.a.mptctc 1.663e+45 8.55

limoneneCI.J.a.lmpmmp 7.243e+45 9.44

limoneneCI.J.a.cptpmm 9.371e+45 9.59

limoneneCI.J.a.mmpmpm 2.961e+45 8.91

limoneneCI.J.a.mttpmm 3.353e+45 8.99

limoneneCI.J.a.cptptm 7.319e+45 9.49

limoneneCI.J.a.ptmpmm 1.626e+45 8.59

limoneneCI.J.a.mptcmc 1.897e+45 8.70

limoneneCI.J.a.ptmptc 1.137e+45 8.40

limoneneCI.J.a.mtpptc 5.895e+45 9.39

limoneneCI.J.a.cppmmp 6.686e+44 8.09

limoneneCI.J.a.ptppmp 5.168e+45 9.34

limoneneCI.J.a.lttmtc 6.476e+45 9.48

limoneneCI.J.a.lttpmp 2.374e+45 8.89

limoneneCI.J.a.cmtpmp 8.961e+45 9.69

limoneneCI.J.a.mttmtc 6.010e+45 9.46

limoneneCI.J.a.ltmppc 5.179e+44 8.02

limoneneCI.J.a.lmtpmc 4.311e+45 9.29

limoneneCI.J.a.cptptc 2.611e+45 9.02

limoneneCI.J.a.ppmctm 2.517e+45 9.00

limoneneCI.J.a.cmtmmp 1.079e+46 9.88

limoneneCI.J.a.pmpmmc 3.029e+45 9.14

limoneneCI.J.a.cptmmm 9.143e+45 9.80

limoneneCI.J.a.cmtpmm 1.204e+46 9.99

limoneneCI.J.a.cmpcpc 8.435e+44 8.43

limoneneCI.J.a.cmpmmp 4.102e+45 9.37

limoneneCI.J.a.mptctp 2.082e+45 8.98

limoneneCI.J.a.cmpmpp 6.783e+44 8.31

limoneneCI.J.a.pmtmmc 6.564e+45 9.67

limoneneCI.J.a.mptcpc 3.603e+44 7.94

limoneneCI.J.a.cmtmmm 1.265e+46 10.06

limoneneCI.J.a.cptmmc 6.357e+45 9.67

limoneneCI.J.a.lttmpm 5.686e+45 9.60

limoneneCI.J.a.cmtmtc 8.594e+45 9.85

limoneneCI.J.a.pptcpm 7.318e+44 8.41

limoneneCI.J.a.lmtpmp 2.930e+45 9.24

limoneneCI.J.a.pmmptp 5.392e+45 9.61

limoneneCI.J.a.lmpmmm 1.258e+46 10.12

limoneneCI.J.a.lptmmc 4.961e+45 9.57

limoneneCI.J.a.mmtmpp 8.836e+45 9.93

limoneneCI.J.a.cppmtp 7.442e+44 8.46

limoneneCI.J.a.mptmtm 3.833e+44 8.10

limoneneCI.J.a.mttmpm 8.340e+45 9.94

limoneneCI.J.a.lmtmmp 2.555e+45 9.27

limoneneCI.J.a.ltmctp 6.056e+45 9.79

limoneneCI.J.a.mpmptm 2.609e+44 7.92

limoneneCI.J.a.lmtmmm 3.459e+45 9.47

limoneneCI.J.a.pptcpp 1.146e+45 8.84

limoneneCI.J.a.mptmmp 1.248e+45 8.89

limoneneCI.J.a.pmtmpm 3.928e+45 9.58

limoneneCI.J.a.lttptp 1.717e+46 10.46

limoneneCI.J.a.ppmpmp 2.143e+45 9.24

limoneneCI.J.a.ptppmm 4.463e+45 9.68

limoneneCI.J.a.mttppm 1.154e+46 10.26

limoneneCI.J.a.pmtppm 3.162e+45 9.50

limoneneCI.J.a.pmpmmp 4.045e+45 9.66

limoneneCI.J.a.pmtppc 9.321e+44 8.79

limoneneCI.J.a.lttmtp 1.399e+46 10.40

limoneneCI.J.a.cpmppp 9.611e+44 8.81

limoneneCI.J.a.ppmpmc 1.081e+45 8.89

limoneneCI.J.a.pmpmmm 6.745e+45 9.98

limoneneCI.J.a.pptcmc 5.960e+45 9.91

limoneneCI.J.a.mmtmpm 1.007e+46 10.23

limoneneCI.J.a.pptmtm 6.733e+44 8.63

limoneneCI.J.a.ltmcpc 2.953e+45 9.54

limoneneCI.J.a.mmpmmm 1.603e+45 9.19

limoneneCI.J.a.lttmpc 4.874e+45 9.85

limoneneCI.J.a.mmtmtc 8.172e+45 10.16

limoneneCI.J.a.pmtpmc 7.524e+45 10.12

limoneneCI.J.a.pmtptc 9.777e+44 8.91

limoneneCI.J.a.pptmpp 1.847e+44 7.95

limoneneCI.J.a.ptmpmc 8.057e+44 8.85

limoneneCI.J.a.mmmpmc 1.806e+45 9.34

limoneneCI.J.a.cptptp 6.621e+45 10.12

limoneneCI.J.a.lttppm 7.176e+45 10.19

limoneneCI.J.a.ppmpmm 2.269e+45 9.52

limoneneCI.J.a.lmtpmm 2.737e+45 9.68

limoneneCI.J.a.ptpptm 4.855e+45 10.02

limoneneCI.J.a.cptcpm 3.343e+45 9.81

limoneneCI.J.a.mmtppm 6.083e+45 10.19

limoneneCI.J.a.ptppmc 2.749e+45 9.72

limoneneCI.J.a.ptmppc 1.218e+45 9.24

limoneneCI.J.a.pmtmtm 4.740e+45 10.06

limoneneCI.J.a.pptctp 8.628e+45 10.43

limoneneCI.J.a.mppmtm 3.253e+44 8.49

limoneneCI.J.a.cmtppc 9.164e+44 9.13

limoneneCI.J.a.pppmtc 3.221e+44 8.52

limoneneCI.J.a.mppmtc 3.211e+44 8.52

limoneneCI.J.a.pppmmc 4.289e+44 8.70

limoneneCI.J.a.lmtppc 1.773e+45 9.54

limoneneCI.J.a.mttpmc 1.380e+46 10.77

limoneneCI.J.a.lppmmc 4.272e+44 8.70

limoneneCI.J.a.lmtmpm 1.122e+46 10.65

limoneneCI.J.a.lmtppm 8.131e+45 10.49

limoneneCI.J.a.mmpmmp 2.175e+45 9.73

limoneneCI.J.a.cttcpp 1.186e+46 10.77

limoneneCI.J.a.ptmppm 7.756e+44 9.16

limoneneCI.J.a.cmtptc 6.917e+45 10.47

limoneneCI.J.a.pptmtc 7.463e+44 9.16

limoneneCI.J.a.cmmptp 3.090e+45 10.06

limoneneCI.J.a.ptmptp 1.865e+45 9.77

limoneneCI.J.a.ppmppp 1.708e+44 8.41

limoneneCI.J.a.cmpmmm 4.383e+45 10.47

limoneneCI.J.a.pptpmc 2.619e+45 10.22

limoneneCI.J.a.mptcmm 3.803e+45 10.44

limoneneCI.J.a.lttppc 5.205e+45 10.66

limoneneCI.J.a.pppmmp 9.357e+44 9.64

limoneneCI.J.a.mptmtc 8.179e+44 9.60

limoneneCI.J.a.mmtptc 5.591e+45 10.75

limoneneCI.J.a.mtpptm 2.571e+45 10.30

limoneneCI.J.a.ptpppp 1.681e+45 10.07

limoneneCI.J.a.ptpptp 6.246e+45 10.86

limoneneCI.J.a.cmpmpm 1.172e+45 9.92

limoneneCI.J.a.mmtptp 1.693e+45 10.15

limoneneCI.J.a.pptmmp 1.177e+46 11.33

limoneneCI.J.a.lmtmtm 3.540e+45 10.64

limoneneCI.J.a.cmtppm 3.644e+45 10.66

limoneneCI.J.a.pptcpc 2.282e+45 10.41

limoneneCI.J.a.lmtptc 1.184e+45 10.05

limoneneCI.J.a.cmtmtm 3.248e+45 10.65

limoneneCI.J.a.cttcpc 4.026e+45 10.84

limoneneCI.J.a.pmtmtp 1.493e+46 11.64

limoneneCI.J.a.pptmmm 9.764e+45 11.45

limoneneCI.J.a.pppmmm 1.051e+45 10.13

limoneneCI.J.a.pptpmp 9.379e+45 11.45

limoneneCI.J.a.pmtmpp 4.061e+45 10.96

limoneneCI.J.a.mmtmpc 4.601e+45 11.04

limoneneCI.J.a.mpmpmc 1.620e+45 10.43

limoneneCI.J.a.pptptm 5.503e+45 11.19

limoneneCI.J.a.mppmtp 4.966e+44 9.75

limoneneCI.J.a.pmmptc 3.435e+45 10.91

limoneneCI.J.a.cppmpp 1.729e+44 9.13

limoneneCI.J.a.pppmtp 4.928e+44 9.76

limoneneCI.J.a.cptmpm 3.785e+44 9.63

limoneneCI.J.a.pmtmpc 6.636e+45 11.36

limoneneCI.J.a.ctpmpc 1.637e+45 10.56

limoneneCI.J.a.mptpmc 2.691e+45 10.87

limoneneCI.J.a.cmtmpp 3.733e+45 11.07

limoneneCI.J.a.pptmmc 3.053e+45 10.97

limoneneCI.J.a.ctpmpp 2.153e+45 10.83

limoneneCI.J.a.cmtmpm 3.205e+45 11.07

limoneneCI.J.a.cptppp 7.453e+44 10.20

limoneneCI.J.a.mmtmtp 1.414e+46 11.97

limoneneCI.J.a.pmtptp 9.550e+45 11.83

limoneneCI.J.a.mptpmp 3.137e+45 11.24

limoneneCI.J.a.mptppm 2.503e+45 11.12

limoneneCI.J.a.pptpmm 6.661e+45 11.80

limoneneCI.J.a.pppmpp 1.834e+44 9.72

limoneneCI.J.a.mptptm 2.805e+45 11.35

limoneneCI.J.a.cmtptp 9.727e+45 12.10

limoneneCI.J.a.cmtmpc 2.693e+45 11.34

limoneneCI.J.a.mptptc 2.104e+45 11.21

limoneneCI.J.a.ltpppm 5.197e+45 11.79

limoneneCI.J.a.mptptp 3.249e+45 11.65

limoneneCI.J.a.mpmpmp 9.035e+44 10.91

limoneneCI.J.a.pptptc 2.251e+45 11.46

limoneneCI.J.a.cmmptc 4.000e+44 10.45

limoneneCI.J.a.mtppmc 3.759e+45 11.92

limoneneCI.J.a.cttppp 3.786e+45 12.11

limoneneCI.J.a.mtpppc 4.298e+45 12.21

limoneneCI.J.a.pptptp 6.074e+45 12.62

limoneneCI.J.a.cttmpp 3.842e+45 12.39

limoneneCI.J.a.cppmpm 3.564e+44 11.04

limoneneCI.J.a.cttmpc 1.805e+45 12.17

limoneneCI.J.a.pptppm 9.144e+44 11.77

limoneneCI.J.a.lptppm 2.813e+45 12.47

limoneneCI.J.a.cttppc 1.885e+45 12.36

limoneneCI.J.a.pptmpm 1.055e+45 12.14

limoneneCI.J.a.pptppp 1.394e+45 12.34

limoneneCI.J.a.mppmpp 4.122e+44 11.64

limoneneCI.J.a.lptmpm 2.765e+45 13.01

limoneneCI.J.a.mppmpm 3.192e+44 11.74

limoneneCI.J.a.mppmmp 3.277e+44 11.77

limoneneCI.J.a.pppmpm 2.174e+44 11.84

Lowest-energy geometries for Limonene-CI-5b and the TS for reaction with H_2O

limoneneCI.J.a.cmpctc

E(RM062X/Aug-CC-pVTZ) (Hartree): -616.16737837

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-1.230217	0.130300	-0.181520
C	-2.732861	0.029131	-0.005297
C	-0.574360	0.931388	0.947673
C	-0.653808	-1.295839	-0.311470
H	-1.048402	0.655851	-1.123343
C	-3.326846	0.050650	1.181558
H	-2.775948	0.171690	2.104890
H	-4.399596	-0.059896	1.268079
C	-3.512720	-0.129631	-1.278639
H	-4.569161	-0.296297	-1.080744
H	-3.411473	0.765658	-1.895800
H	-3.137856	-0.965288	-1.872403

C	0.785832	-1.406347	-0.803308
H	-0.741731	-1.788918	0.658369
H	-1.290698	-1.846655	-1.003435
C	1.851179	-1.204323	0.256052
H	0.963276	-2.408575	-1.206457
H	0.993467	-0.720009	-1.628816
O	1.571498	-1.136474	1.432938
C	3.258964	-1.057485	-0.240130
H	3.963249	-1.236205	0.567118
H	3.454023	-1.719902	-1.082667
H	3.362693	-0.024973	-0.593993
C	0.770946	1.467858	0.641917
H	-1.198480	1.794024	1.210043
H	-0.475080	0.332195	1.854185
O	1.141647	1.600256	-0.532733
H	1.477040	1.776991	1.409817
O	2.414109	2.095730	-0.753437

Rotational constants (GHz): 1.2369800 0.5100100 0.4501500

Vibrational harmonic frequencies (cm-1):

30.5905	61.1015	75.2827
107.8194	137.5643	146.5638
150.8098	177.2846	190.4817
192.5662	242.0582	253.5988
288.6198	316.7628	341.9295
363.0045	438.7731	475.0502
489.2926	513.6987	553.3115
612.7749	655.3926	726.3878
764.2280	783.6377	840.3162
875.8259	907.3622	936.5060
950.9856	968.3052	984.7993
1002.1290	1006.7188	1036.6772
1058.2336	1062.9948	1085.3860
1109.6015	1136.3520	1188.3072
1214.2452	1247.7428	1262.1564
1298.1917	1327.6798	1342.2657
1378.8579	1384.3729	1391.3439
1410.7764	1417.0164	1433.1876
1444.9409	1453.0084	1459.2353
1473.4730	1477.5595	1481.8263
1489.8237	1497.6268	1672.4173
1742.9787	1813.4683	3031.0941
3034.9004	3050.6060	3053.8056
3056.8254	3076.6912	3091.5580
3107.9541	3110.7304	3120.3735
3121.1925	3151.7312	3168.1651
3169.6239	3178.4981	3248.1822

Zero-point correction (Hartree): 0.246327

limoneneCI.J.a.lmpctc

E(RM062X/Aug-CC-pVTZ) (Hartree): -616.16715894

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-1.225655	-0.020848	-0.262811
C	-2.729737	-0.134198	-0.097149
C	-0.665524	0.688919	0.985410
C	-0.544392	-1.368708	-0.528505
H	-1.047303	0.628797	-1.125089
C	-3.334483	-1.237580	0.324297
H	-2.792804	-2.145098	0.551434
H	-4.408750	-1.264753	0.451462
C	-3.500068	1.110222	-0.436137
H	-4.555666	1.004135	-0.196450
H	-3.113929	1.981622	0.097267
H	-3.405944	1.331089	-1.501487
C	0.910435	-1.298780	-0.982635
H	-0.594421	-1.987179	0.369244
H	-1.124064	-1.875518	-1.300018
C	1.932329	-1.156958	0.127903
H	1.179022	-2.220570	-1.508287
H	1.080392	-0.494273	-1.703670
O	1.621505	-1.263359	1.294206
C	3.335128	-0.841080	-0.298827
H	4.033239	-1.074370	0.499823
H	3.599644	-1.367437	-1.215134
H	3.366800	0.234607	-0.508643
C	0.646326	1.353802	0.811847
H	-1.355890	1.466565	1.332494
H	-0.565962	-0.020963	1.807926
O	1.036020	1.680278	-0.317835
H	1.308661	1.592445	1.641505
O	2.273827	2.288351	-0.420463

Rotational constants (GHz): 1.2362200 0.5353900 0.4325500

Vibrational harmonic frequencies (cm-1):

30.1840	58.7148	69.4821
116.7122	134.7996	139.5322
149.2154	178.2601	184.8170
203.7937	243.0001	243.6464
277.5144	311.6968	345.8258
380.3661	441.3482	462.3596
491.5530	522.2804	548.6803
615.0296	654.0787	733.6254
762.4280	780.7759	830.3642
874.2246	909.5924	935.7397
957.3259	967.9793	987.3748
996.7813	1013.0919	1026.6992
1056.9187	1073.7331	1077.2889
1112.4571	1137.5118	1189.3262
1215.1577	1239.6721	1269.5524
1295.7346	1321.2452	1350.8149

1367.5915	1387.0416	1404.4995
1411.3379	1415.9436	1416.6353
1435.8311	1454.2068	1454.9768
1473.3656	1480.9246	1487.0380
1488.9483	1496.9488	1670.3296
1744.2488	1812.8799	3031.1063
3039.9608	3050.8086	3051.8804
3054.5318	3074.0329	3089.1780
3103.5379	3109.4065	3120.4875
3120.7338	3151.7083	3166.0008
3173.5470	3178.5718	3255.2147

Zero-point correction (Hartree): 0.246251

limoneneCI.J.a.pmpctc

E(RM062X/Aug-CC-pVTZ) (Hartree): -616.16778842

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-1.215211	0.166005	-0.298580
C	-2.723449	0.091411	-0.181466
C	-0.629767	0.740432	1.003192
C	-0.634915	-1.212944	-0.661290
H	-0.986340	0.859741	-1.109476
C	-3.502966	0.824996	-0.965900
H	-3.087821	1.490858	-1.711754
H	-4.581553	0.780430	-0.887141
C	-3.287922	-0.842524	0.851305
H	-4.371570	-0.761839	0.896785
H	-3.031901	-1.878589	0.623914
H	-2.887261	-0.628003	1.844286
C	0.830270	-1.230040	-1.084246
H	-0.757665	-1.893276	0.183226
H	-1.237151	-1.605178	-1.482137
C	1.830325	-1.234651	0.055243
H	1.040217	-2.137330	-1.659644
H	1.076854	-0.398920	-1.750440
O	1.483102	-1.404583	1.203667
C	3.261024	-0.982820	-0.317548
H	3.921282	-1.311327	0.479810
H	3.515906	-1.466622	-1.259763
H	3.367366	0.099507	-0.457634
C	0.719244	1.338000	0.883647
H	-1.281964	1.533336	1.390751
H	-0.567360	-0.021755	1.781699
O	1.161868	1.673436	-0.223688
H	1.367760	1.518887	1.738591
O	2.432705	2.215258	-0.270881

Rotational constants (GHz): 1.2338100 0.5267700 0.4447200

Vibrational harmonic frequencies (cm-1):

35.8737	44.2115	66.7715

108.3728	134.7193	137.8884
145.1249	174.1954	191.8817
197.7844	230.1991	239.1409
280.2627	298.2164	334.7704
377.6376	442.6552	471.4668
498.3891	514.6126	553.1991
615.6013	655.0476	742.6666
765.3691	780.5568	828.2731
871.2706	889.9190	935.7109
958.0546	966.7902	986.1688
998.6867	1014.0446	1033.1508
1058.3675	1071.0884	1079.0476
1113.7354	1128.6016	1189.4242
1212.9125	1244.9573	1290.0920
1302.4442	1321.2755	1332.7649
1373.4099	1384.8692	1397.5499
1408.9397	1414.2705	1420.1793
1441.6287	1448.1774	1458.7627
1473.3648	1481.0532	1483.4511
1491.0918	1498.8396	1671.4299
1743.7624	1812.5961	3027.4844
3030.2635	3050.0469	3058.6559
3067.5783	3081.1348	3088.9108
3105.3455	3111.7665	3117.4905
3120.8319	3151.8615	3161.1846
3167.5616	3178.2823	3244.5465

Zero-point correction (Hartree): 0.246110

limoneneCI+H2O.J.a.cmpctcmdu

E(RM062X/Aug-CC-pVTZ) (Hartree): -692.60689791

Electronic state : 1-A

Cartesian coordinates (Angs):

C	1.421678	-0.031030	-0.232972
C	2.916651	-0.158725	0.003537
C	0.645207	-1.165824	0.470296
C	1.015650	1.396631	0.196453
H	1.254470	-0.117283	-1.310244
C	3.431621	-0.612286	1.139344
H	2.812247	-0.961973	1.955363
H	4.502114	-0.643851	1.292697
C	3.780064	0.321608	-1.126597
H	4.833618	0.314967	-0.856146
H	3.641184	-0.314587	-2.003389
H	3.506920	1.335186	-1.427568
C	-0.309107	1.925617	-0.336567
H	1.014385	1.439117	1.286779
H	1.802172	2.072831	-0.139739
C	-1.531736	1.457140	0.412683

H	-0.325453	3.018956	-0.269406
H	-0.447737	1.689694	-1.393525
O	-1.438466	0.934143	1.506237
C	-2.856071	1.658460	-0.256836
H	-3.655635	1.656279	0.479299
H	-2.870007	2.577741	-0.840611
H	-2.997154	0.814967	-0.943311
C	-0.594625	-1.625201	-0.225701
H	1.287772	-2.039879	0.567393
H	0.364011	-0.865596	1.481522
O	-1.142897	-0.838731	-1.063466
H	-0.789373	-2.683512	-0.355731
O	-2.425902	-1.359557	-1.426391
O	-2.082702	-1.713024	1.051944
H	-2.616569	-1.634361	0.192482
H	-2.113226	-0.839681	1.475707

Rotational constants (GHz): 1.0146700 0.4588000 0.3998500

Vibrational harmonic frequencies (cm-1):

i327.0986	60.3489	70.5215
87.4564	129.0759	137.3019
148.3951	161.7680	181.9230
192.5778	208.1490	222.6944
242.4065	257.7823	304.2962
318.2646	340.4124	375.3744
444.2631	480.8571	492.3237
504.5471	518.8028	558.5032
615.2857	634.5096	665.2323
726.6531	766.8066	778.3312
809.1952	849.5198	895.9735
910.6529	951.5511	960.7534
979.9547	992.3921	1007.3126
1035.9885	1054.6532	1066.5734
1082.4235	1095.5824	1127.5959
1136.6175	1159.6313	1198.5106
1222.4531	1245.7163	1263.6114
1301.5993	1332.3845	1336.0490
1369.5762	1383.6013	1392.5627
1412.1218	1415.3235	1423.6696
1447.7744	1452.4439	1465.6921
1473.0807	1477.0706	1484.6739
1488.8212	1496.6266	1562.0516
1637.1370	1743.0661	1797.8984
2880.1326	3028.4087	3046.5264
3052.1508	3056.9420	3077.4490
3083.5774	3100.5654	3104.3482
3119.2148	3122.1016	3127.0966
3151.5056	3165.1362	3172.9744
3184.9956	3244.6417	3710.4646

Zero-point correction (Hartree): 0.273364

limoneneCI+H2O.J.a.mmpctcmdu

E(RM062X/Aug-CC-pVTZ) (Hartree): -692.60693989

Electronic state : 1-A

Cartesian coordinates (Angs):

C	1.417559	0.142510	-0.275014
C	2.915644	0.041940	-0.046943
C	0.744460	-0.873614	0.690593
C	0.897666	1.580766	-0.145554
H	1.230031	-0.191629	-1.299810
C	3.597679	0.895621	0.705858
H	3.132070	1.746735	1.183173
H	4.660063	0.766021	0.865511
C	3.578624	-1.123366	-0.723909
H	4.623166	-1.214059	-0.434405
H	3.074001	-2.063157	-0.488313
H	3.527269	-1.005403	-1.808457
C	-0.472928	1.849066	-0.754656
H	0.879127	1.874213	0.905328
H	1.618818	2.227925	-0.644667
C	-1.649660	1.448837	0.100190
H	-0.594884	2.922890	-0.933594
H	-0.586173	1.371005	-1.729896
O	-1.514994	1.196500	1.281904
C	-2.983631	1.370905	-0.576596
H	-3.783178	1.462077	0.153907
H	-3.079967	2.129221	-1.352330
H	-3.043398	0.385051	-1.052985
C	-0.437652	-1.606577	0.145090
H	1.463839	-1.627873	1.007341
H	0.428537	-0.349917	1.593992
O	-1.060902	-1.087524	-0.835740
H	-0.527293	-2.680424	0.264005
O	-2.287354	-1.795134	-1.042710
O	-1.910926	-1.539102	1.445473
H	-2.451142	-1.708224	0.604226
H	-2.024046	-0.598905	1.661196

Rotational constants (GHz): 0.9993100 0.4764300 0.3934200

Vibrational harmonic frequencies (cm-1):

i327.0284	59.4176	66.6032
85.2731	127.9206	147.0318
148.9141	162.6874	177.8000
190.8380	203.5120	231.5576
241.1646	261.4321	301.2697
321.1121	350.8457	398.2758
448.4142	464.0970	493.2636
502.4968	523.7800	555.7561
616.8052	631.0363	658.7578
733.6452	764.7980	776.4740
816.8723	843.6337	892.0674

916.1953	956.8130	961.9349
977.7912	999.5320	1006.2147
1027.0309	1057.0739	1072.4942
1077.5641	1093.8930	1125.8823
1130.6710	1160.8057	1199.2536
1223.8759	1240.0804	1271.7451
1296.1874	1325.2248	1348.7209
1359.4047	1385.4672	1394.4817
1413.1261	1417.4154	1421.9874
1448.4378	1454.1645	1462.8542
1472.9923	1484.4221	1487.3108
1489.9904	1498.1633	1561.1353
1635.2418	1743.3510	1797.1956
2892.9786	3031.2692	3047.2119
3049.9255	3052.8048	3076.2376
3090.1669	3099.0177	3102.3389
3121.0612	3121.9360	3128.6418
3149.7223	3170.9443	3172.2505
3184.0611	3252.1253	3708.5736

Zero-point correction (Hartree): 0.273483

limoneneCI+H2O.J.a.pmpctcmdu

E(RM062X/Aug-CC-pVTZ) (Hartree): -692.60803453

Electronic state : 1-A

Cartesian coordinates (Angs):

C	1.408320	0.009035	-0.364470
C	2.907414	-0.114681	-0.181794
C	0.717615	-1.021257	0.567770
C	0.981290	1.472810	-0.143504
H	1.183624	-0.258495	-1.398438
C	3.684519	-0.544199	-1.167838
H	3.275574	-0.812923	-2.133552
H	4.755180	-0.638490	-1.039594
C	3.459840	0.271249	1.160886
H	4.524746	0.058667	1.221534
H	3.312180	1.335727	1.351105
H	2.954975	-0.266624	1.966381
C	-0.385127	1.862057	-0.691689
H	1.013068	1.707902	0.921605
H	1.730952	2.097575	-0.632077
C	-1.553812	1.483351	0.184130
H	-0.444635	2.949756	-0.806762
H	-0.559058	1.447050	-1.686597
O	-1.391710	1.152271	1.342810
C	-2.913327	1.526223	-0.442406
H	-3.678745	1.623403	0.323051
H	-2.989562	2.332226	-1.170801
H	-3.051702	0.574512	-0.969248
C	-0.529108	-1.641033	0.026255

H	1.405754	-1.840463	0.779300
H	0.467079	-0.560345	1.524854
O	-1.149736	-1.026594	-0.900300
H	-0.683571	-2.712143	0.086937
O	-2.426731	-1.641658	-1.097953
O	-1.951432	-1.557600	1.378534
H	-2.526619	-1.644311	0.545681
H	-1.998113	-0.625698	1.647841

Rotational constants (GHz): 1.0069700 0.4661700 0.4032400

Vibrational harmonic frequencies (cm-1):

i330.7710	59.0542	68.2997
86.5882	132.0942	139.3530
149.9426	160.0444	179.0866
190.2524	199.5511	221.2631
244.2037	255.2949	305.1449
306.6236	339.1656	397.4995
445.5381	483.2211	499.9509
506.2658	519.6503	561.3273
618.3646	633.8692	663.1895
742.8709	769.7887	779.0448
810.6855	847.6674	879.1623
904.5541	955.5719	958.9035
982.1367	997.4819	1010.0814
1033.6370	1060.8988	1073.0904
1076.0328	1097.4974	1121.6298
1135.0661	1161.7743	1201.0900
1223.1423	1249.8212	1291.1411
1296.6869	1320.1087	1338.2904
1364.1398	1382.4395	1395.8323
1403.7527	1416.8216	1421.5206
1450.3178	1457.3543	1462.6828
1472.9555	1482.9661	1485.6938
1491.3811	1498.3741	1560.5095
1636.7711	1743.5738	1797.0057
2864.7928	3030.7281	3047.7852
3056.5819	3067.8163	3076.4215
3083.0580	3098.5769	3107.7361
3117.0973	3121.5305	3122.4510
3151.7473	3160.7230	3171.7975
3186.6419	3243.9764	3708.7703

Zero-point correction (Hartree): 0.273437