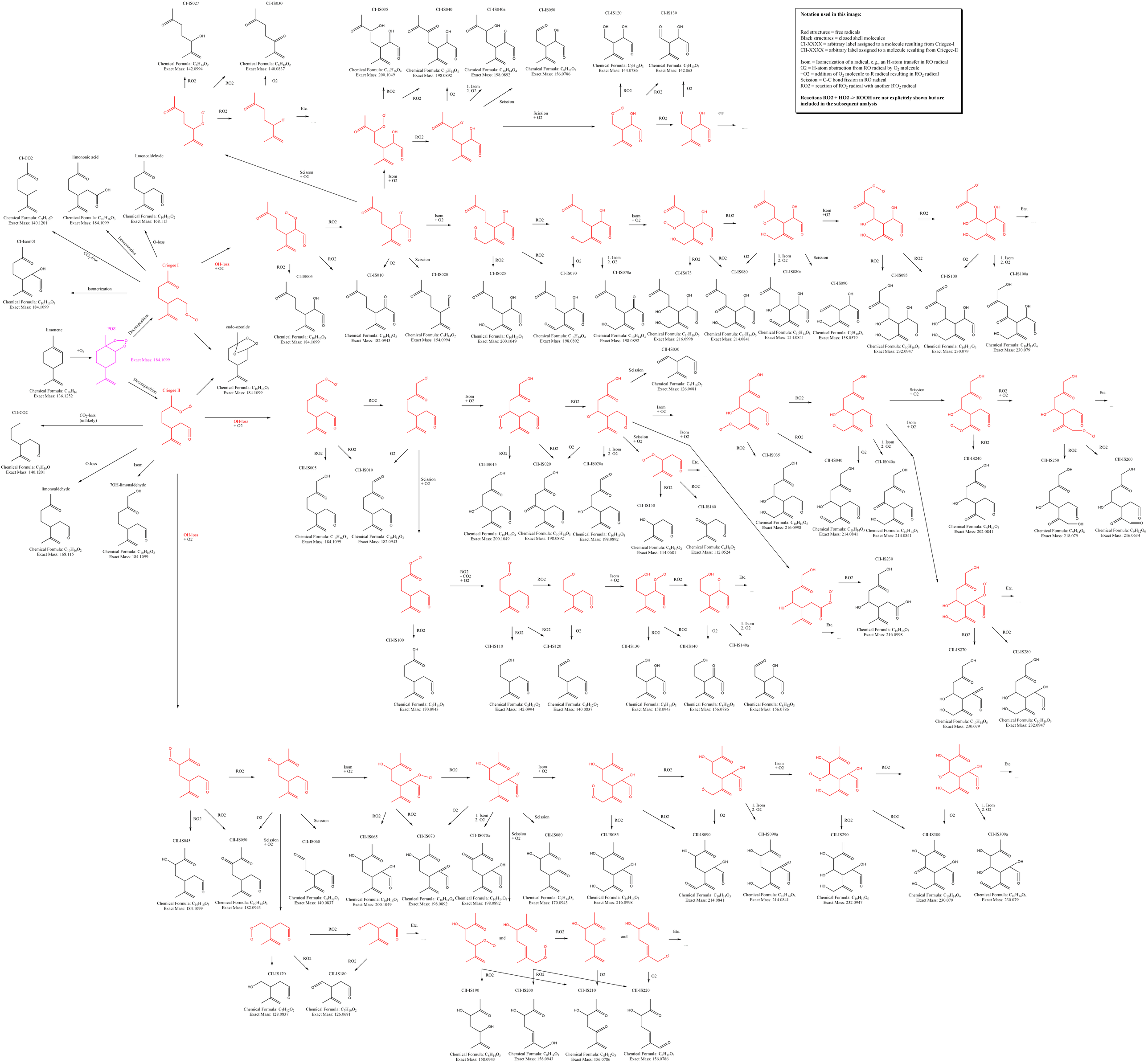
Notation used in this image:
Red structures = free radicals
Black structures = closed shell molecules
CI-XXXX = arbitrary label assigned to a molecule resulting from Criegee-I
CII-XXXX = arbitrary label assigned to a molecule resulting from Criegee-II
Isom = Isomerization of a radical, e.g., an H-atom transfer in RO radical
O2 = H-atom abstraction from RO radical by O2 molecule
+O2 = addition of O2 molecule to R radical resulting in RO2 radical
Scission = C-C bond fission in RO radical
RO2 = reaction of RO2 radical with another R'O2 radical
Reactions RO2 + HO2 -> ROOH are not explicitely shown but are included in the subsequent analysis
limonene
+O3
POZ
Exact Mass: 184.1099
Decomposition
Criegee I
Criegee II
OH-loss + O2
endo-ozonide
Chemical Formula: C10H16
Exact Mass: 136.1252
Chemical Formula: C10H10O3
Exact Mass: 184.1099
CO2-loss
CO2-loss (unlikely)
Isomerization
O-loss
Isom
CI-CO2
CI-Isom01
limononic acid
limonoaldehyde
7OH-limonaldehyde
Chemical Formula: C9H14O
Exact Mass: 140.1201
Chemical Formula: C10H18O3
Exact Mass: 184.1099
Chemical Formula: C10H18O2
Exact Mass: 168.115
CII-CO2
Chemical Formula: C9H16O
Exact Mass: 140.1201
Chemical Formula: C10H16O2
Exact Mass: 168.115
Chemical Formula: C10H16O3
Exact Mass: 184.1099
CI-IS027
CI-IS030
CI-IS035
CI-IS040
CI-IS040a
CI-IS050
CI-IS120
CI-IS130
Chemical Formula: C9H14O2
Exact Mass: 142.0994
Chemical Formula: C8H12O2
Exact Mass: 140.0837
Chemical Formula: C10H16O4
Exact Mass: 200.1049
Chemical Formula: C10H14O4
Exact Mass: 198.0892
Chemical Formula: C8H12O3
Exact Mass: 156.0786
Chemical Formula: C7H12O3
Exact Mass: 144.0786
Chemical Formula: C7H10O3
Exact Mass: 142.063
RO2
O2
Isom + O2
1. Isom 2. O2
Scission
Scission + O2
Etc.
CI-IS005
CI-IS010
CI-IS020
CI-IS025
CI-IS070
CI-IS070a
CI-IS075
CI-IS080
CI-IS080a
CI-IS090
CI-IS095
CI-IS100
CI-IS100a
Chemical Formula: C10H10O3
Exact Mass: 184.1099
Chemical Formula: C10H14O3
Exact Mass: 182.0943
Chemical Formula: C9H12O2
Exact Mass: 154.0994
Chemical Formula: C10H14O4
Exact Mass: 200.1049
Chemical Formula: C10H14O4
Exact Mass: 198.0892
Chemical Formula: C10H14O5
Exact Mass: 214.0841
Chemical Formula: C7H10O4
Exact Mass: 158.0579
Chemical Formula: C10H10O6
Exact Mass: 232.0947
Chemical Formula: C10H14O6
Exact Mass: 230.079
CII-IS005
CII-IS010
CII-IS015
CII-IS020
CII-IS020a
CII-IS030
CII-IS035
CII-IS040
CII-IS040a
CII-IS150
CII-IS160
CII-IS240
CII-IS250
CII-IS260
Chemical Formula: C7H10O2
Exact Mass: 126.0681
Chemical Formula: C10H16O5
Exact Mass: 216.0998
Chemical Formula: C9H16O2
Exact Mass: 114.0681
Chemical Formula: C9H8O2
Exact Mass: 112.0524
Chemical Formula: C9H14O5
Exact Mass: 202.0841
Chemical Formula: C9H16O6
Exact Mass: 218.079
Chemical Formula: C9H12O6
Exact Mass: 216.0634
CII-IS100
CII-IS110
CII-IS120
CII-IS130
CII-IS140
CII-IS140a
CII-IS230
CII-IS270
CII-IS280
RO2 - CO2 + O2
Chemical Formula: C9H14O3
Exact Mass: 170.0943
Chemical Formula: C8H14O2
Exact Mass: 142.0994
Chemical Formula: C8H12O2
Exact Mass: 140.0837
Chemical Formula: C9H16O3
Exact Mass: 158.0943
Chemical Formula: C8H14O3
Exact Mass: 156.0786
Chemical Formula: C8H12O3
Exact Mass: 156.0786
CII-IS045
CII-IS050
CII-IS060
CII-IS065
CII-IS070
CII-IS070a
CII-IS080
CII-IS085
CII-IS090
CII-IS090a
CII-IS290
CII-IS300
CII-IS300a
CII-IS170
CII-IS180
CII-IS190
CII-IS200
CII-IS210
CII-IS220
and
Chemical Formula: C7H12O2
Exact Mass: 128.0837
Chemical Formula: C7H10O2
Exact Mass: 126.0681