Supplementary Information

# Characterizing highly oxygenated organic molecules in limonene secondary organic aerosol: roles of temperature and relative humidity

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The SI includes: 2 figures and 2 tables.

**Table S1.** The twenty most abundant HOM products from the ozonolysis of lomonene at T = 25°C and 5°C as well as RH = 15% and 75%. Note that all compounds are deteced as clusters with $Na^+$ adducts.

| T = 25°C | | T = 5°C | | RH = 15% | | RH = 75% | |
|---|---|---|---|---|---|---|---|
| Formula | *m/z* | Formula | *m/z* | Formula | *m/z* | Formula | *m/z* |
| $C_{20}H_{34}O_8$ | 425.2146 | $C_{20}H_{34}O_8$ | 425.2146 | $C_{19}H_{30}O_9$ | 425.1781 | $C_{19}H_{32}O_9$ | 427.1937 |
| $C_{10}H_{16}O_6$ | 255.0839 | $C_{20}H_{34}O_9$ | 441.2095 | $C_{19}H_{32}O_8$ | 411.1988 | $C_{19}H_{32}O_8$ | 411.1988 |
| $C_{19}H_{32}O_8$ | 411.1989 | $C_{19}H_{32}O_8$ | 411.1989 | $C_{19}H_{30}O_8$ | 409.1832 | $C_{20}H_{34}O_8$ | 425.2145 |
| $C_{19}H_{30}O_8$ | 409.1833 | $C_{19}H_{30}O_8$ | 409.1833 | $C_{19}H_{32}O_9$ | 427.1937 | $C_{19}H_{30}O_9$ | 425.1781 |
| $C_{20}H_{34}O_9$ | 441.2095 | $C_{10}H_{16}O_6$ | 255.0839 | $C_{19}H_{30}O_{10}$ | 441.1730 | $C_{18}H_{30}O_9$ | 413.1781 |
| $C_{19}H_{30}O_9$ | 425.1782 | $C_{20}H_{34}O_7$ | 409.2196 | $C_{10}H_{16}O_6$ | 255.0838 | $C_{20}H_{34}O_9$ | 441.2094 |
| $C_{20}H_{32}O_9$ | 439.1938 | $C_{19}H_{30}O_9$ | 425.1782 | $C_{19}H_{32}O_7$ | 395.2039 | $C_{19}H_{30}O_8$ | 409.1832 |
| $C_{19}H_{32}O_7$ | 395.2040 | $C_{19}H_{32}O_9$ | 427.1938 | $C_{19}H_{30}O_7$ | 393.1883 | $C_{19}H_{32}O_{10}$ | 443.1886 |
| $C_{20}H_{34}O_{10}$ | 457.2044 | $C_{20}H_{32}O_9$ | 439.1938 | $C_{19}H_{32}O_{10}$ | 443.1886 | $C_{19}H_{30}O_{10}$ | 441.1730 |
| $C_{10}H_{18}O_6$ | 257.0995 | $C_{19}H_{32}O_7$ | 395.204 | $C_{18}H_{30}O_8$ | 397.1831 | $C_{19}H_{32}O_7$ | 395.2039 |
| $C_{20}H_{32}O_8$ | 423.1989 | $C_{20}H_{32}O_8$ | 423.1989 | $C_{18}H_{28}O_9$ | 411.1624 | $C_{20}H_{34}O_7$ | 409.2196 |
| $C_{20}H_{32}O_{10}$ | 455.1887 | $C_{20}H_{34}O_{10}$ | 457.2044 | $C_{18}H_{28}O_8$ | 395.1674 | $C_{19}H_{32}O_9$ | 439.1938 |
| $C_{20}H_{34}O_7$ | 409.2196 | $C_{20}H_{32}O_{10}$ | 455.1887 | $C_{19}H_{30}O_{11}$ | 457.1679 | $C_{18}H_{30}O_8$ | 397.1833 |
| $C_{19}H_{32}O_{10}$ | 443.1887 | $C_{19}H_{30}O_7$ | 393.1884 | $C_{18}H_{30}O_9$ | 413.1781 | $C_{20}H_{32}O_{10}$ | 455.1888 |
| $C_{19}H_{30}O_7$ | 393.1884 | $C_{20}H_{32}O_7$ | 407.2040 | $C_{18}H_{28}O_{10}$ | 427.1573 | $C_{18}H_{28}O_9$ | 411.1624 |
| $C_{19}H_{30}O_{10}$ | 441.1731 | $C_{19}H_{30}O_{10}$ | 441.1731 | $C_{18}H_{30}O_7$ | 381.1883 | $C_{18}H_{30}O_{10}$ | 429.1730 |
| $C_{18}H_{30}O_8$ | 397.1833 | $C_{19}H_{32}O_{10}$ | 443.1887 | $C_{18}H_{30}O_{10}$ | 429.1730 | $C_{10}H_{16}O_6$ | 255.0839 |
| $C_{18}H_{30}O_9$ | 413.1782 | $C_{20}H_{34}O_{11}$ | 473.1993 | $C_{18}H_{28}O_7$ | 379.1726 | $C_{20}H_{34}O_{10}$ | 457.2044 |
| $C_{20}H_{32}O_7$ | 407.204 | $C_{18}H_{30}O_8$ | 397.1833 | $C_{19}H_{30}O_6$ | 377.1933 | $C_{18}H_{30}O_7$ | 381.1883 |
| $C_{20}H_{34}O_{11}$ | 473.1993 | $C_{19}H_{30}O_{11}$ | 457.1680 | $C_{19}H_{32}O_{11}$ | 459.1836 | $C_{20}H_{32}O_{10}$ | 455.1887 |

**Table S2.** Singlal intensity in each volatility class in the ozonolysis of lomonene at T = 25℃ and 5℃ as well as RH = 15% and 75%. Note that "-" in the table means no monomer is classified into ELOVC or ULVOC.

| | SVOC | LVOC | ELVOC | ULVOC |
|---|---|---|---|---|
| **Temperature conditions** | | | | |
| T = 5℃ | | | | |
| Monomer | 1.03E10 | 1.58E09 | - | - |
| Dimer | 4.20E09 | 7.02E10 | 2.66E10 | 9.33E08 |
| T = 25℃ | | | | |
| Monomer | 1.18E10 | 4.81E09 | - | - |
| Dimer | 4.90E09 | 5.94E10 | 2.38E10 | 2.38E08 |
| **RH conditions** | | | | |
| RH = 15% | | | | |
| Monomer | 4.06E10 | 9.47E08 | - | - |
| Dimer | 6.90E09 | 4.28E11 | 1.67E11 | 1.17E09 |
| RH = 75% | | | | |
| Monomer | 3.84E10 | 8.66E08 | - | - |
| Dimer | 6.20E09 | 4.96E11 | 1.92E11 | 1.13E09 |

**Figure S1.** The (a) formula number and (b) intensity molecular weight distributons ;imonene SOA at T = 25℃ and 5℃ and RH = 15% and 75%.

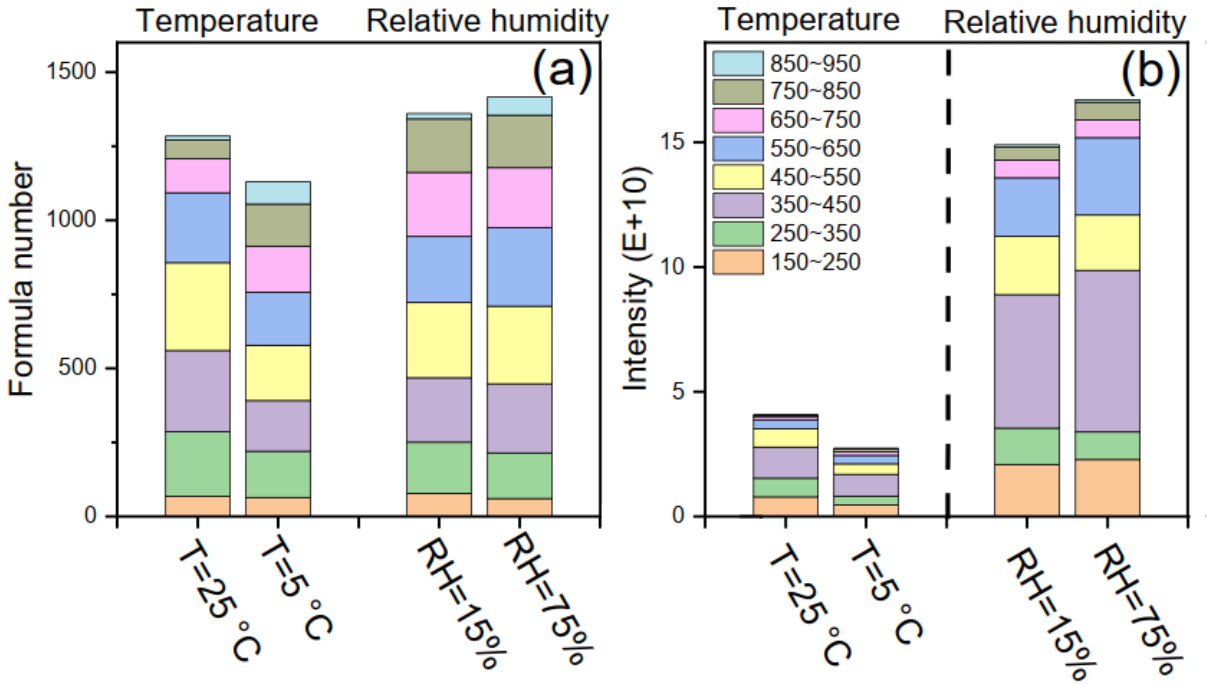

**Figure S2.** Potential reaction pathways to form the larger molecules through (a) hydroperoxide + carbonyl channels, (b) alcohol + carbonyl, and (c) peroxycarboxylic acid + carbonyl channels.