Supporting Information for

Secondary organic aerosol formation from 2-methyl-3-buten-2-ol (MBO) photooxidation: Evidence for acid-catalyzed reactive uptake of epoxides

Haofei Zhang[1, †], Zhenfa Zhang[1], Tianqu Cui[1], Ying-Hsuan Lin[1], Neil A. Bhathela[1], John Ortega[2], David R. Worton[3,4], Allen H. Goldstein[3,5], Alex Guenther[2, ‡], Jose L. Jimenez[6], Avram Gold[1], and Jason D. Surratt[1,*]

[1] Department of Environmental Sciences and Engineering, Gillings School of Global Public Health, The University of North Carolina at Chapel Hill, Chapel Hill, North Carolina, USA.

[2] National Center for Atmospheric Research, Atmospheric Chemistry Division, Boulder, Colorado, USA.

[3] Department of Environmental Science, Policy and Management, University of California, Berkeley, California, USA.

[4] Aerosol Dynamics Inc., Berkeley, CA, 94710, USA.

[5] Department of Civil and Environmental Engineering, University of California, Berkeley, California, USA.

[6] Cooperative Institute for Research in Environmental Sciences, and Department of Chemistry and Biochemistry, University of Colorado, Boulder, Colorado, USA.

[†] Now at Department of Environmental Science, Policy and Management, University of California, Berkeley, California, USA.

[‡] Now at Atmospheric Sciences and Global Change, Pacific Northwest National Laboratory, Richland, Washington, USA.

[*] Corresponding author: J. D. Surratt, Department of Environmental Sciences and Engineering, Gillings School of Global Public Health, The University of North Carolina at Chapel Hill, Chapel Hill, NC 27599, USA. (surratt@unc.edu)

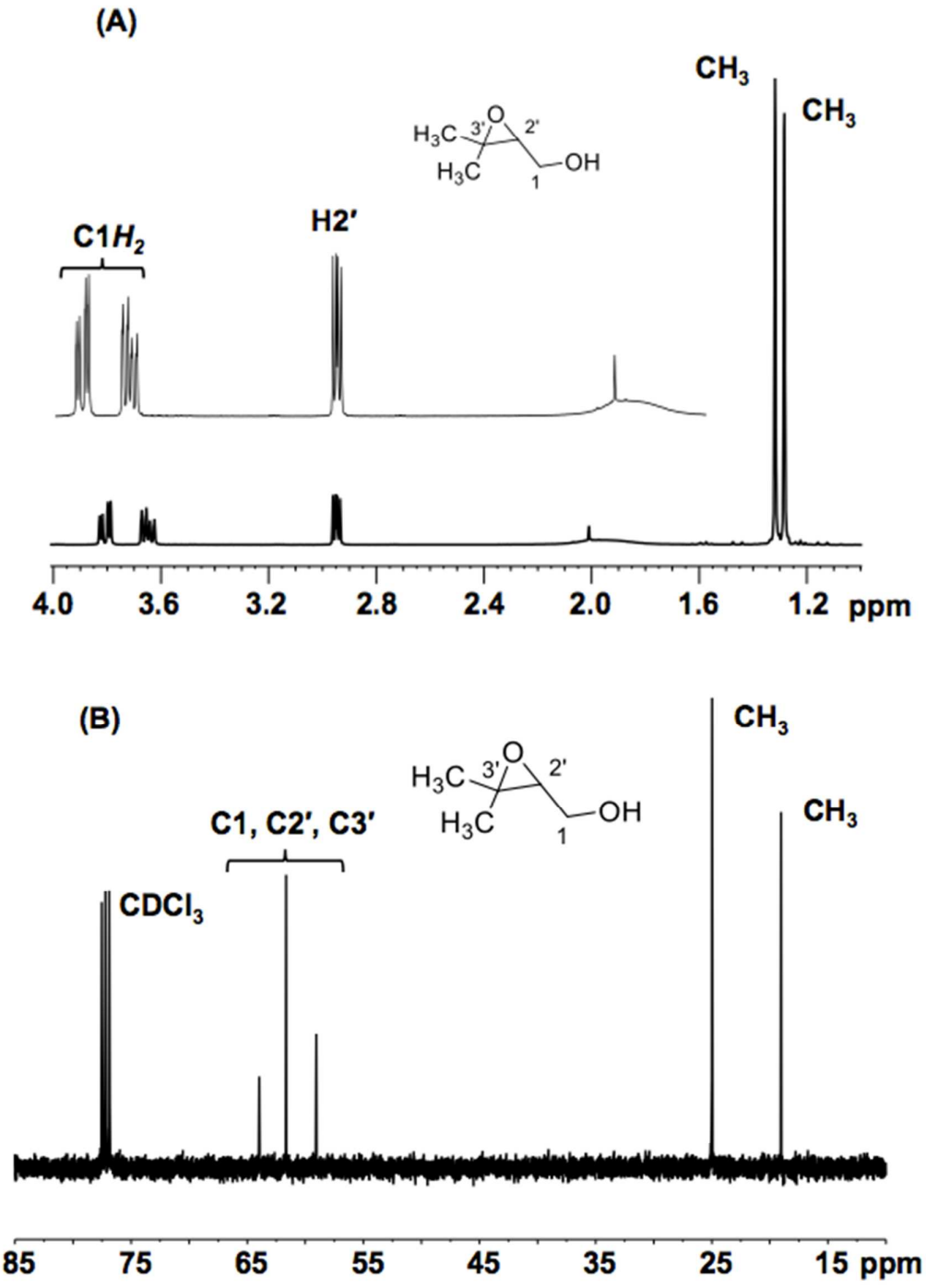

Figure S1. NMR of synthetic MBO epoxide ((3,3-dimethyloxiran-2-yl)methanol). (A) ^{1}H-NMR (40 MHz, $CDCl_3$); (B) ^{13}C-NMR (100 MHz, $CDCl_3$).

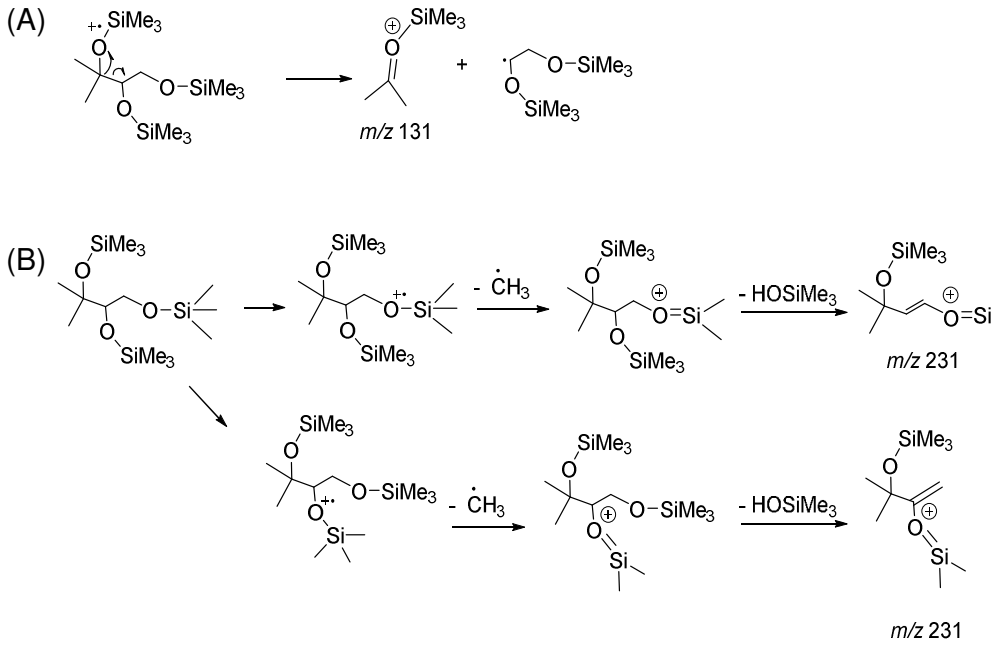

Figure S2. Fragmentation Scheme proposed for product ions (A) *m/z* 131 and (B) *m/z* 231 in the GC/EI-MS of TMS derivatized DHIP.

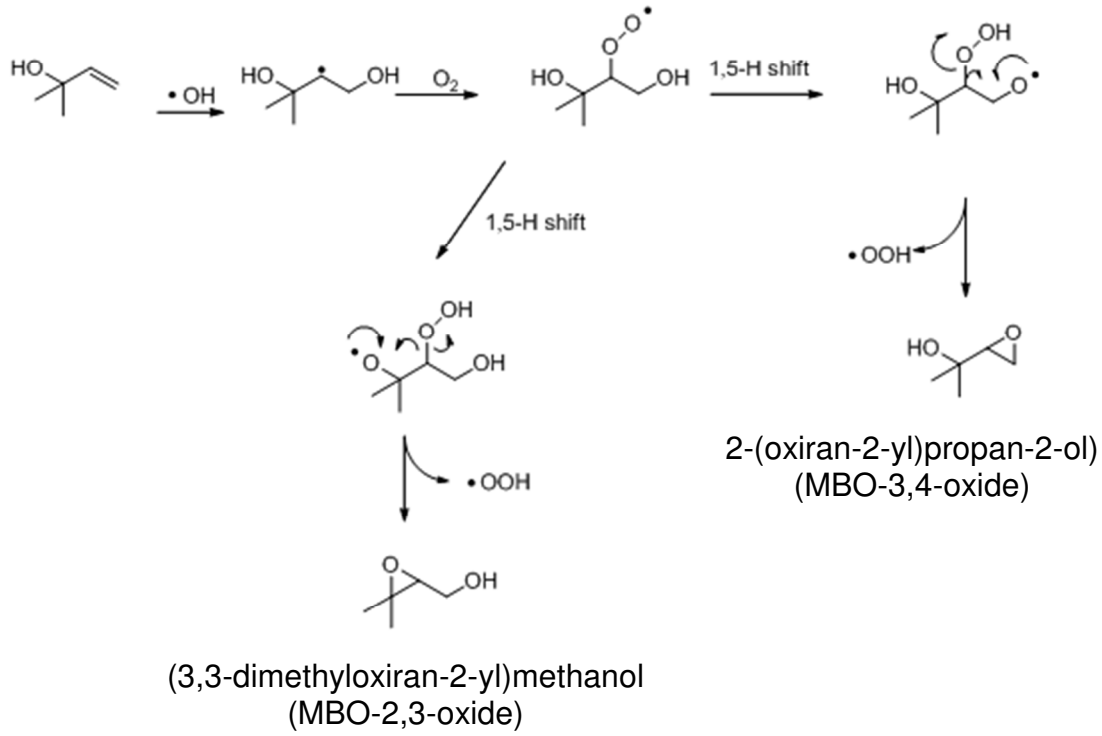

Figure S3. Proposed mechanism leading to formation of isomeric MBO epoxides. The first two steps in this scheme follow the proposed mechanism for isoprene epoxydiols (IEPOX) to yield a hydroxyperoxy radical. The peroxy radical undergoes a 1,5-H shift followed by elimination of HO2. As the scheme indicates, two isomers of MBO oxide are predicted.