

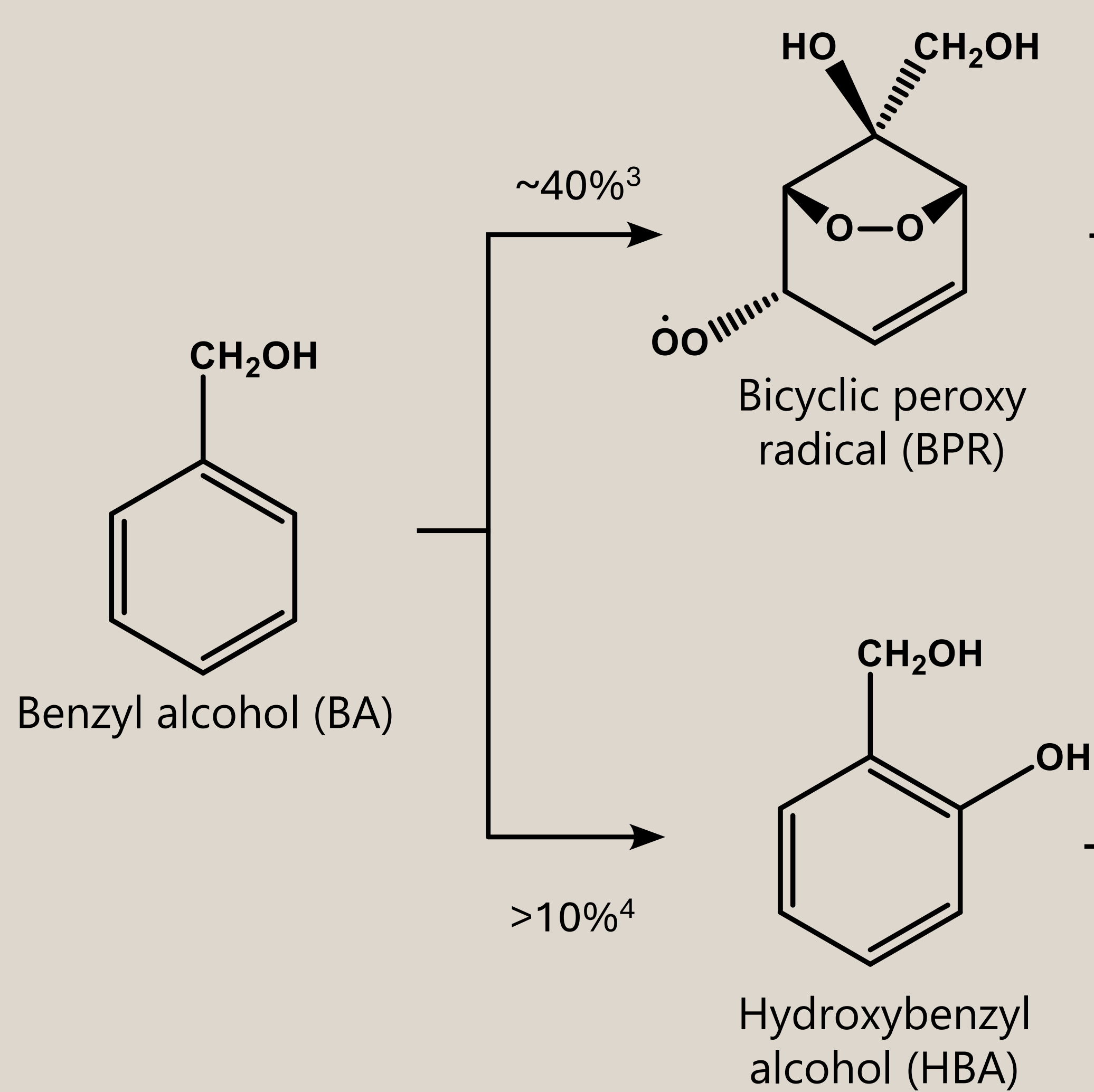
Multigenerational Oxidation of Benzyl Alcohol in the Atmosphere

A. Kervinen¹ and S. Iyer¹

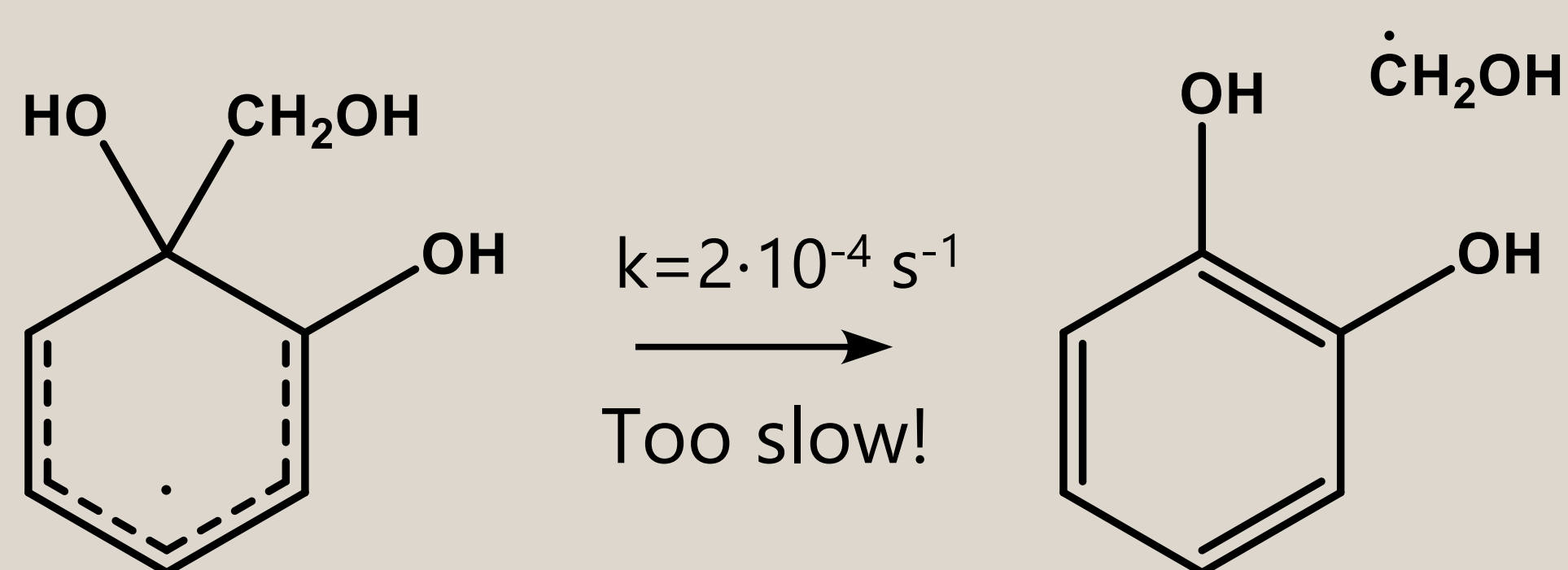
¹Aerosol Physics Laboratory, Tampere University, Finland

Benzyl Alcohol

- Common aromatic VOC
- Found in volatile chemical products (VCPs)¹
 - Cosmetics, inks, dyes and flowers
- Efficient precursor to SOA², likely due to their potential to form HOM
- Understanding the chemistry leads to better SOA estimates



Mechanism to catechol missing

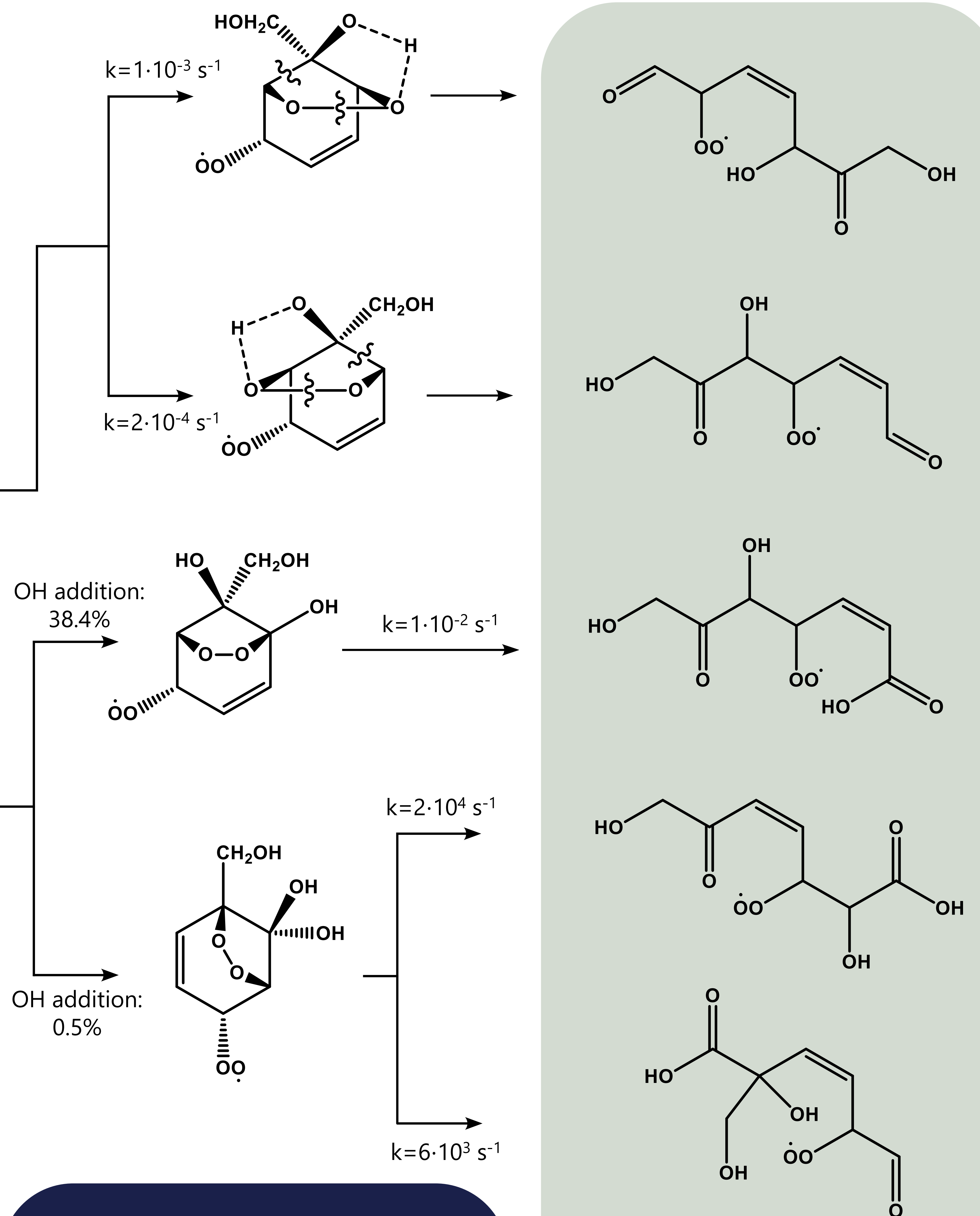


Methods

- Conformer sampling: MMFF
- Opt + freq: ω B97X-D/aug-cc-pVTZ
 - OH reactions: M062-X/aug-cc-pVTZ
- SP: ROHF-RCCSD(T)- F12a/VDZ
- Rate coefficients: MC-TST

References

- [1] McDonald, B. C. et al. (2018) Volatile chemical products emerging as largest petrochemical source of urban organic emissions. *Science*. 359 (6377), 760–764.
- [2] Charan, S. M. et al. (2020) Secondary organic aerosol yields from the oxidation of benzyl alcohol. *Atmospheric chemistry and physics*. 20 (21), 13167–13190.
- [3] Wang, L. (2015) The Atmospheric Oxidation Mechanism of Benzyl Alcohol Initiated by OH Radicals: The Addition Channels. *Chemphyschem*. 16 (7), 1542–1550.
- [4] Buenconsejo, R. S. et al. (2025) Quantifying primary oxidation products in the OH-initiated reaction of benzyl alcohol. *Atmospheric chemistry and physics*. 25 (3), 1883–1897.



Conclusions

- Slow pathway found to HOM from BA
- Faster pathway found to HOM from HBA, important product of BA oxidation
- BPR ring-break is an important pathway for HOM formation

Autoxidation

HOM



Acknowledgements: This project has received funding from the Research Council of Finland project 355966 and Jane and Aatos Erkkon Foundation project 250017. We also thank the CSC IT Center for Science in Espoo, Finland, for the computing resources