Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics. This journal is © the Owner Societies 2015

Electronic Supplementary Information for

Gas-phase reaction of two unsaturated ketones with Cl atom and O₃:

kinetics and products

Jing Wang^{a,b}, Li Zhou^{a,b}, Weigang Wang^{a*}, MaofaGe^{a*}

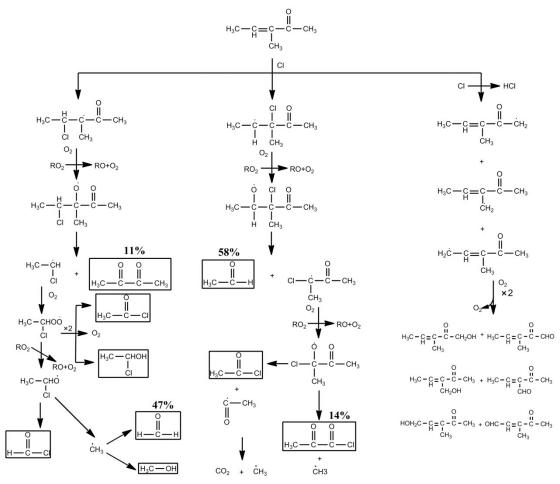
^aBeijing National Laboratory for Molecular Sciences (BNLMS), State Key Laboratory for Structural Chemistry of Unstable and Stable Species, Institute of Chemistry, Chinese Academy of Sciences, Zhongguancun, Beijing 100190, China; ^bUniversity of Chinese Academy of Sciences, Beijing, 100049, China.

1. The Calibration of PTR-MS

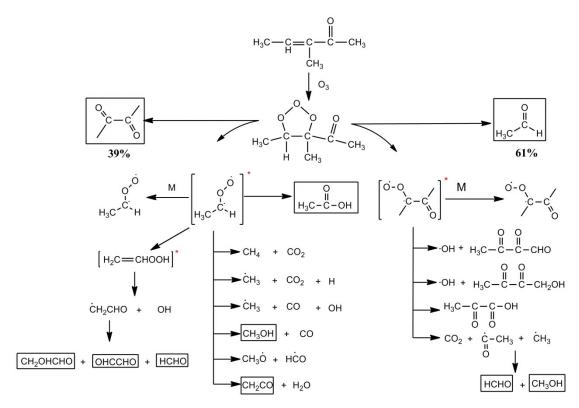
We made calibrations for the two reactants (MBO332 and MPO332) and the five products: formaldehyde, acetaldehyde, formic acid, methanol and 2, 3-butanedione. They were calibrated by the commercial standards in the PTR-MS using the Teflon bags¹.

The concentrations of compounds for which pure commercial standards were not available were determined by the measured rate constants of the proton transfer reactions^{2,3}. For the products without measured rate constants, an estimated rate constant (k) of 2×10^{-9} cm³ molecule⁻¹ s⁻¹ was used. The rate constants for the proton transfer reaction of most compounds are generally within $\pm20\%$ of the estimated k.

Scheme S1. Proposed Reaction pathways for the reaction of MPO332 with C1 atom Scheme S2. Proposed reaction pathways of MPO332 with O₃



Scheme S1. Proposed Reaction pathways for the reaction of MPO332 with Cl atom



Scheme S2. Proposed reaction pathways of MPO332 with O₃

Reference

- 1. A. Lee, A. H. Goldstein, M. D. Keywood, S. Gao, V. Varutbangkul, R. Bahreini, N. L. Ng, R. C. Flagan and J. H. Seinfeld, *J. Geophys. Res.-Atmos.*, 2006, **111**.
- 2. W. Lindinger and A. Jordan, *Chem. Soc. Rev.*, 1998, **27**, 347-375.
- 3. J. Zhao and R. Zhang, Atmos. Environ., 2004, **38**, 2177-2185.