

Supplement of

Oxygenated products formed from OH-initiated reactions of trimethylbenzene: Autoxidation and accretion

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Contents of this file:

4 pages

Table S1

Figures S1-S3

Table S1 Relative abundance of the C9 and C18 oxidation products formed from TMB oxidation (Exp. #1-3 in Table 1), as measured by Nitrate CI-API-TOF. The percentages mean the relative intensity of this compound family to the total signals of detected C9 and C18 products with correction of the relative transmission efficiency of Nitrate CI-API-TOF obtained by the previously reported depletion method (Heinritzi et al., 2016). All of these products, except for C₉H₁₄O₅ that was detected in the 1,2,4-TMB and 1,2,3-TMB experiments, have more than 6 oxygen atoms, which meet the definition of HOMs from Bianchi et al (2019).

Compound Family	1,3,5-TMB	1,2,4-TMB	1,2,3-TMB
C ₉ H ₁₂ O ₆₋₁₁	1.9 %	6.6 %	7.5 %
C ₉ H ₁₄ O ₅₋₁₁	5.9 %	10.2 %	18.3 %
C ₉ H ₁₆ O ₆₋₁₀	5.7 %	9.6 %	11.8 %
C ₁₈ H ₂₄ O ₈₋₁₃	3.2 %	4.9 %	4.0 %
C ₁₈ H ₂₆ O ₈₋₁₅	33.4 %	23.1 %	26.5 %
C ₁₈ H ₂₈ O ₉₋₁₅	44.9 %	39.0 %	26.9 %
C ₁₈ H ₃₀ O ₁₂₋₁₅	5.1 %	6.6 %	5.0 %

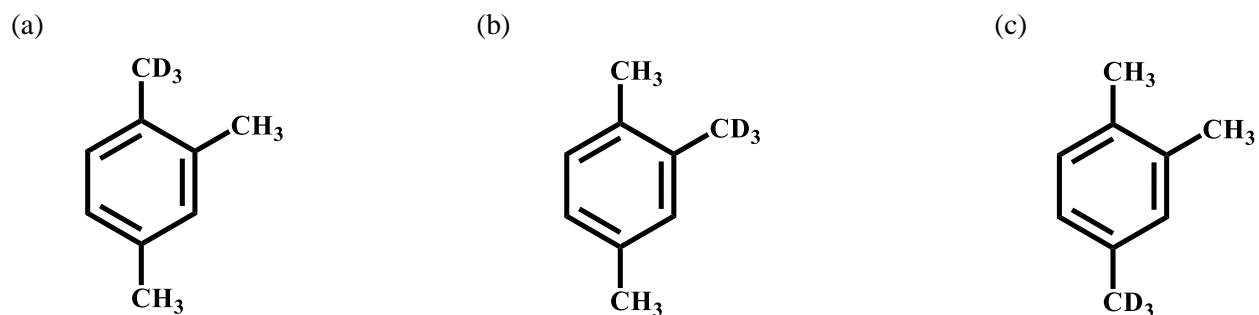


Figure S1. Molecular structure of three partially deuterated precursors. (a) 1,2,4-(1-methyl-D3)-TMB; (b) 1,2,4-(2-methyl-D3)-TMB; and (c) 1,2,4-(4-methyl-D3)-TMB.

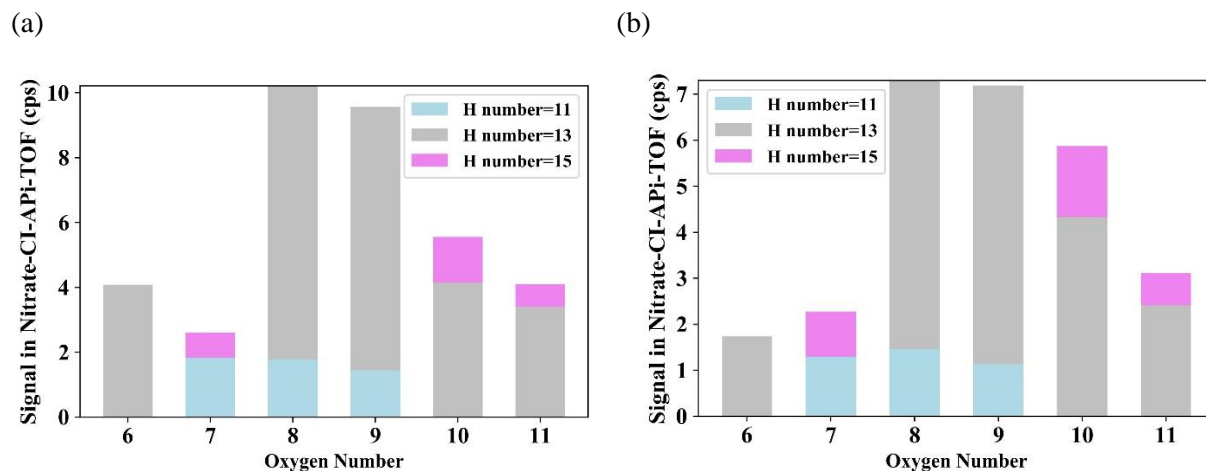
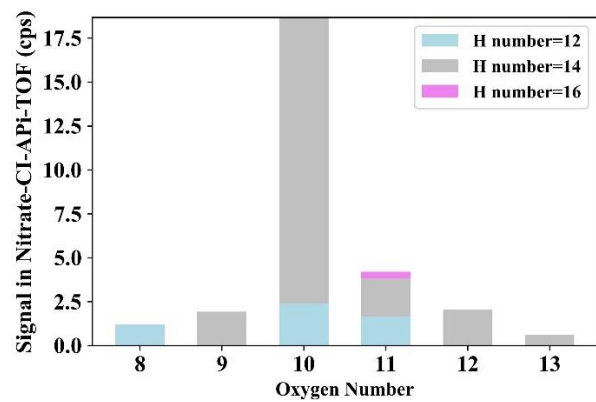


Figure S2. (a) Distribution of $C_9H_xN_1O_y$ formed from 1,2,4-TMB under low NO_x conditions, as detected by Nitrate Cl-API-TOF; and (b) Distribution of $C_9H_xN_1O_y$ formed from 1,2,4-TMB under higher NO_x conditions, as detected by Nitrate Cl-API-TOF.

(a)



(b)

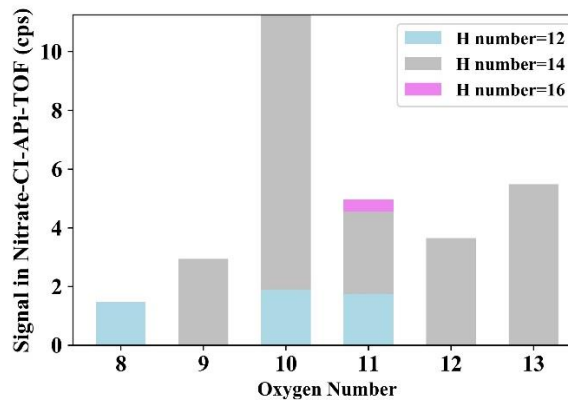


Figure S3. (a) Distribution of $C_9H_xN_2O_y$ formed from 1,2,4-TMB under low NO_x conditions, as detected by Nitrate CI-API-TOF; and (b) Distribution of $C_9H_xN_2O_y$ formed from 1,2,4-TMB under higher NO_x conditions, as detected by Nitrate CI-API-TOF.