

Supplementary Information

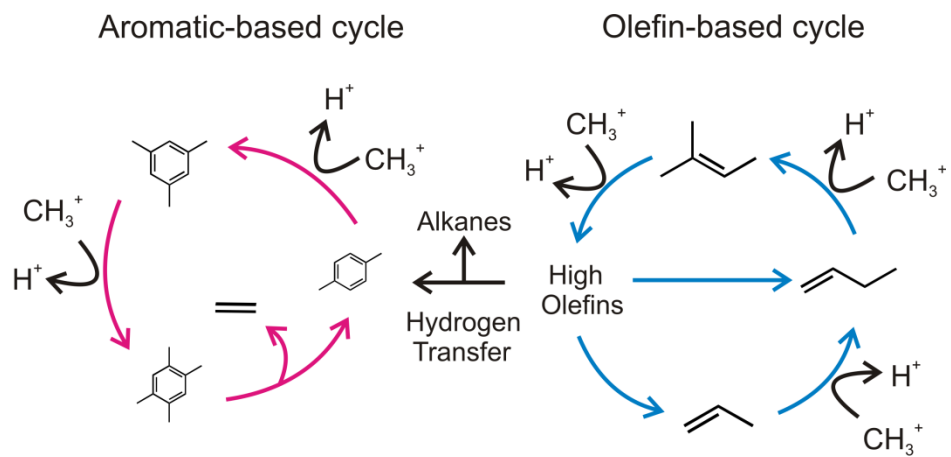
Oxygen-containing Coke Species in Zeolite-catalyzed Conversion of Methanol to Hydrocarbons

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Scheme S1 Dual aromatic- and olefin-based catalytic cycles for the conversion of methanol to hydrocarbons on zeolite catalysts.¹

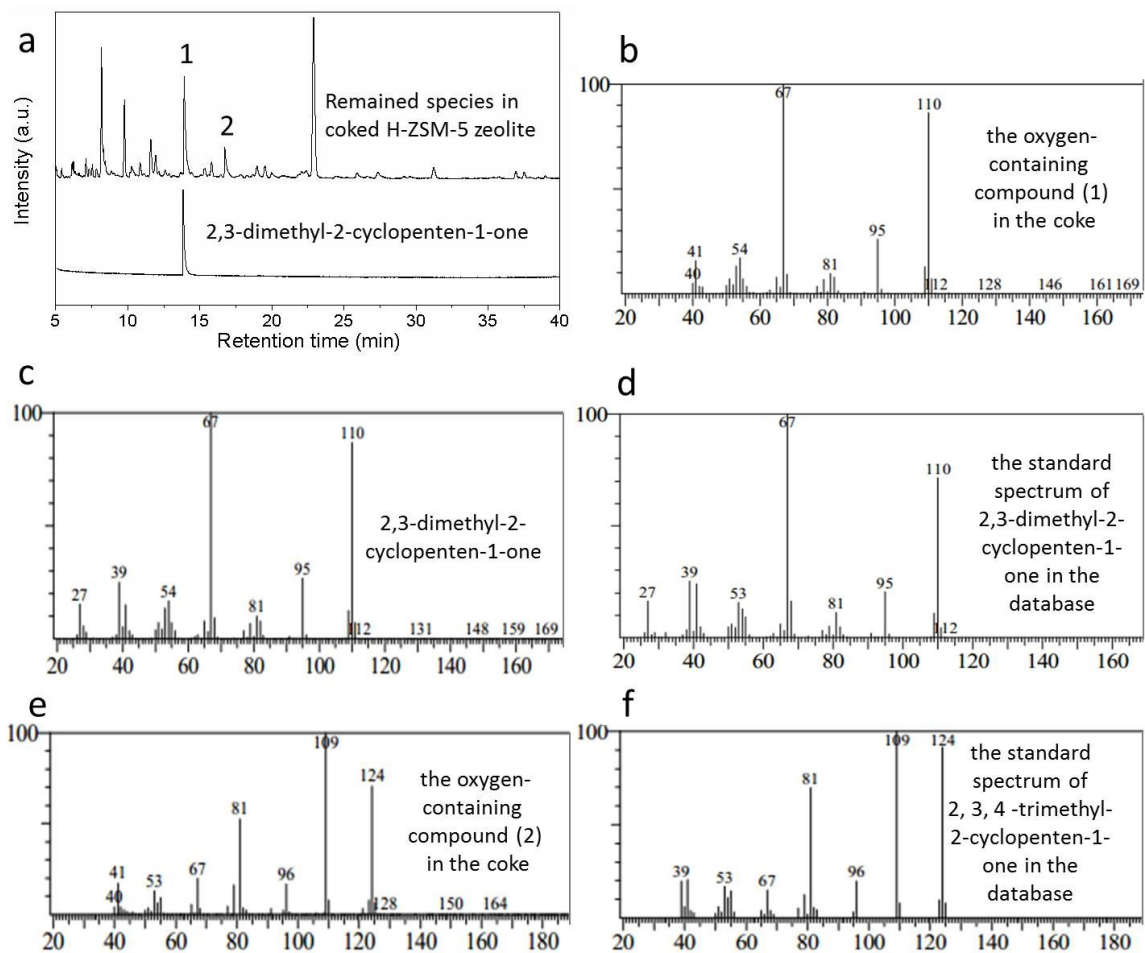


Fig. S1 (a) GC-MS elution profiles of residual species in coked H-ZSM-5 (Si/Al = 25) zeolite (upper) and 2,3-dimethyl-2-cyclopenten-1-one standard sample (lower) under the same GC conditions. (b)-(f) MS spectra of the oxygen-containing compound (1) in the coke (b), 2,3-dimethyl-2-cyclopenten-1-one (c), the standard spectrum of 2,3-dimethyl-2-cyclopenten-1-one in the database (d), the oxygen-containing compound (2) in the coke (e), and the standard spectrum of 2,3,4-trimethyl-2-cyclopenten-1-one in the database (f). The good agreement between the spectra of the identified compounds with those of standard sample and database records validates the assignments of the compounds.

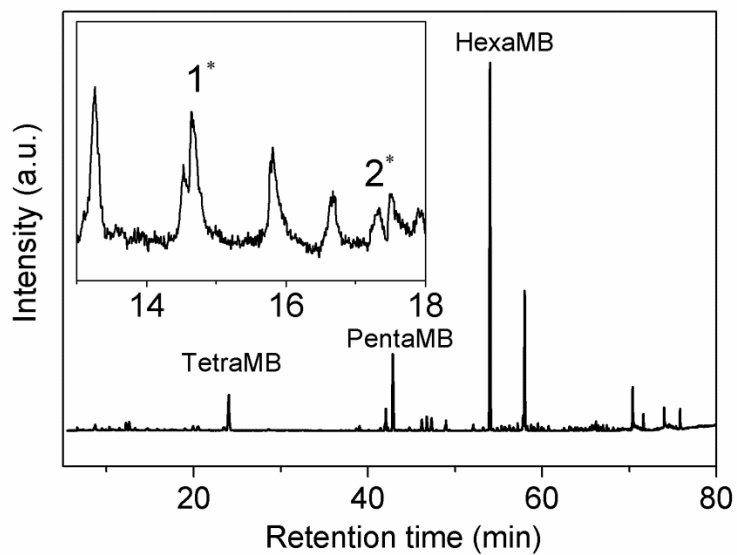


Fig. S2 The GC-MS elution profile of the residual soluble coke species extracted from the used H-ZSM-5 catalyst with a high Si/Al ratio of 150. The inset shows the enlarged profile of the region where oxygenates are present. 1* and 2* label 2,3-dimethyl-2-cyclopenten-1-one and 2,3,4-tri-methyl-2-cyclopenten-1-one, respectively.

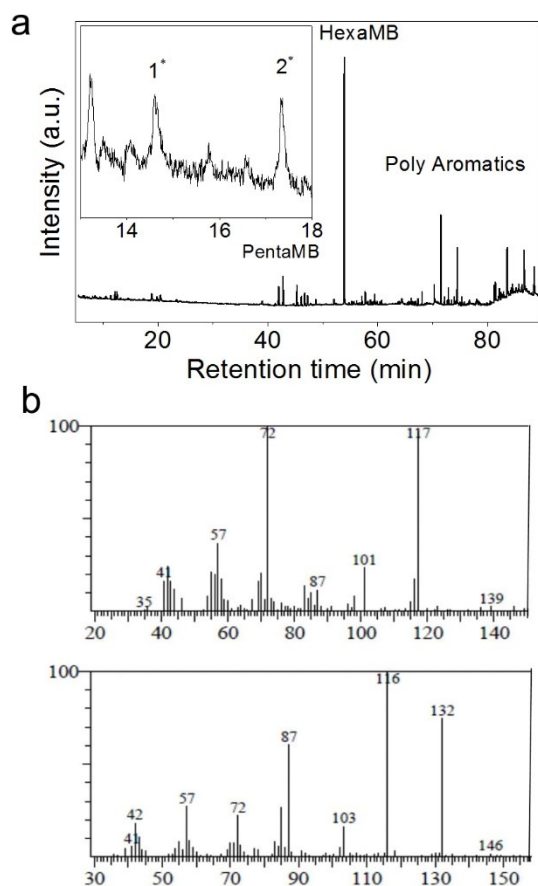
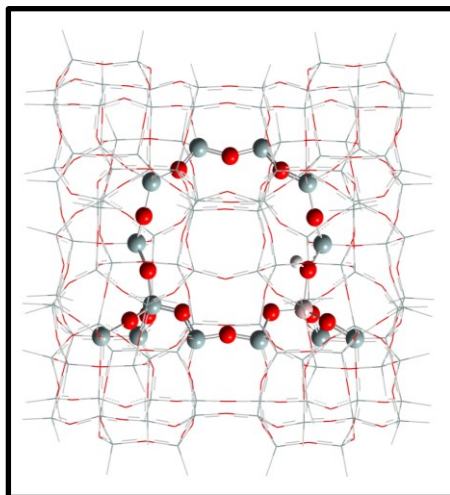


Fig. S3 (a) The GC-MS elution profile of the residual soluble coke species extracted from the H-Beta catalyst (Si/Al=12.5) using ^{13}C -MeOH as the feed. The inset shows the enlarged profile of the region where oxygenates are present. 1* and 2* label 2, 3-dimethyl-2-cyclopenten-1-one and 2,3,4-tri-methyl-2-cyclopenten-1-one, respectively. (b) MS spectra of the extracted 2, 3-dimethyl-2-cyclopenten-1-one (top) and 2, 3, 4-trimethyl-2-cyclopenten-1-one (bottom).

The figure below shows the cluster model of H-ZSM-5 subdivided into two ONIOM layers: the inner 14T cluster (balls) was computed with the B3LYP/6-31G(d,p) level of theory, and the remainder (lines) was treated with the universal force field (UFF) method (Gray: silicon, Red: oxygen, Pink: aluminum, White: hydrogen).²⁻⁵



References

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