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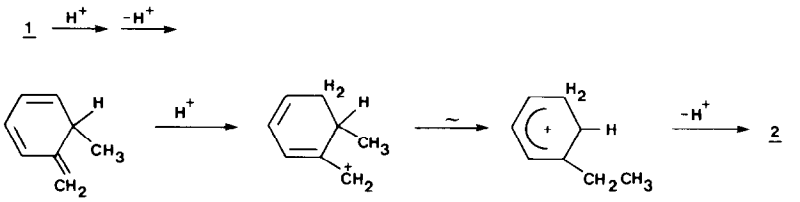
LETTERS TO THE EDITORS

Comments on the Interpretation of the Mechanism of Aromatic Hydrocarbon Participation in the Production of Hydrocarbons from Methanol over ZSM-5 Zeolite

Recently Mole and co-workers reported that simple aromatic hydrocarbons accelerate the conversion of methanol to hydrocarbons over ZSM-5 zeolite (*1*).

The authors observed that a feed composed of ^{13}C-labeled benzene or toluene and methanol affords mono-^{13}C-labeled ethylene and ^{13}C-labeled C_3 hydrocarbons (*2*). They also described the deuteration of toluene and *p*-xylene by D_2O in which some of the deuterium was in the methyl groups.

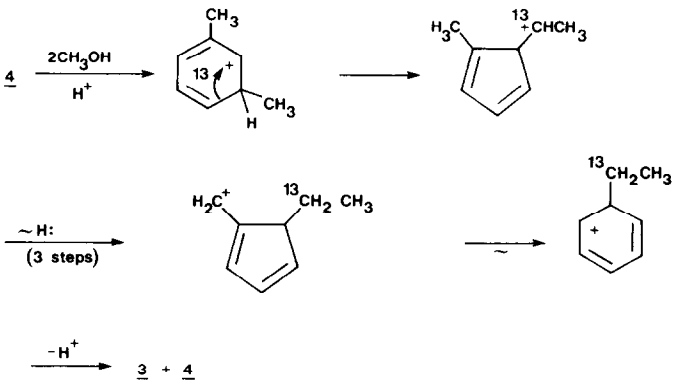
The authors, recognizing that the deethylation of ethyl aromatics might be one of the routes to ethylene formation, considered two mechanisms, of which one involves the isomerization of *o*-xylene (**1**) to ethylbenzene (**2**) via an unusual 1,3-carbon–carbon methyl shift:



The above mechanism would not account for the formation of ^{13}C-labeled ethylene from ^{13}C-labeled benzene and methanol.

The 6,5-ring expansion mechanism also considered by the authors, and used previously to explain the interconversion of xylenes and ethylbenzene (*3*), explains all the ^{13}C and H tracer results.

The formation of mono-^{13}C-labeled ethylene (**3**) from ^{13}C-labeled benzene (**4**) and methanol could be interpreted as



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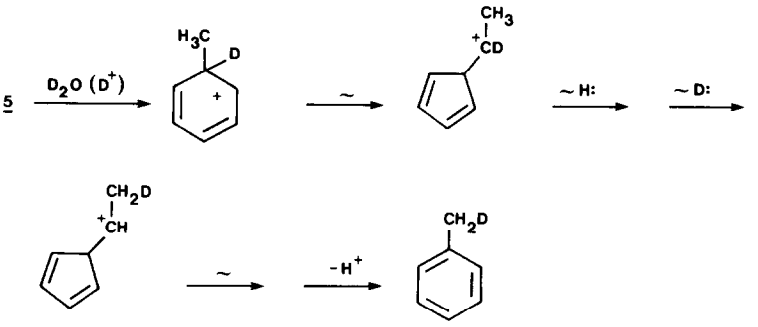
The incorporation of deuterium from D_2O into methyl groups of toluene (**5**) can also be explained by means of ring expansion and contraction steps:



Intramolecular 1,2-carbon–carbon hydride transfers to form tertiary, secondary, and primary cations are common in hydrocarbon conversion reactions, and explain among other things the reversible conversion of cyclohexane to methylcyclopentane and isobutane to butane.

REFERENCES

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2. Mole, T., Bett, G., and Seddon, D., *J. Catal.* **84,** 425 (1983).
3. Pines, H., "The Chemistry of Catalytic Hydrocarbon Conversions," Chap. 1, p. 29. Academic Press, New York, 1981.

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