THERMAL DECOMPOSITION OF C_7H_7 RADICALS; BENZYL, TROPYL, AND NORBORNADIENYL

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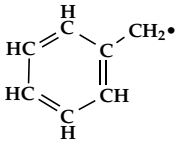
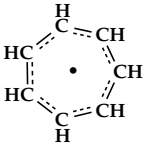
Benzyl radical ($C_6H_5CH_2$) and two other C_7H_7 radicals are commonly encountered in the combustion of substituted aromatic compounds found in biofuels and gasoline. High temperature pyrolysis of benzyl radical requires isomerization to other C_7H_7 radicals that may include cycloheptatrienyl (tropyl) radical (*cyc*-C_7H_7) and norbornadienyl radical. The thermal decomposition of all three radicals has now been investigated using a micro-reactor that heats dilute gas-phase samples up to 1600 K and has a residence time of about 100 μ-sec. The pyrolysis products exit the reactor into a supersonic expansion and are detected using synchrotron-based photoionization mass spectrometry and matrix-isolation IR spectroscopy. The products of the pyrolysis of benzyl radical ($C_6H_5CH_2$) along with three isotopomers ($C_6H_5^{13}CH_2$, $C_6D_5CH_2$, and $C_6H_5CD_2$) were detected and identified[a]. The distribution of ^{13}C atoms and D atoms indicate that multiple different decomposition pathways are active.

[a]Buckingham, G. T., Ormond, T. K., Porterfield, J. P., Hemberger, P., Kostko, O., Ahmed, M., Robichaud, D. J., Nimlos, M. R., Daily, J. W., Ellison, G. B. 2015, Journal of Chemical Physics **142** 044307



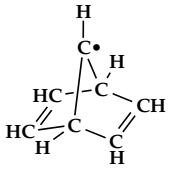
benzyl radical

$\tilde{X}\ ^2B_1$



tropyl radical

$\tilde{X}\ ^2E_2''$



norboradienyl radical

$\tilde{X}\ ^2B_1$