

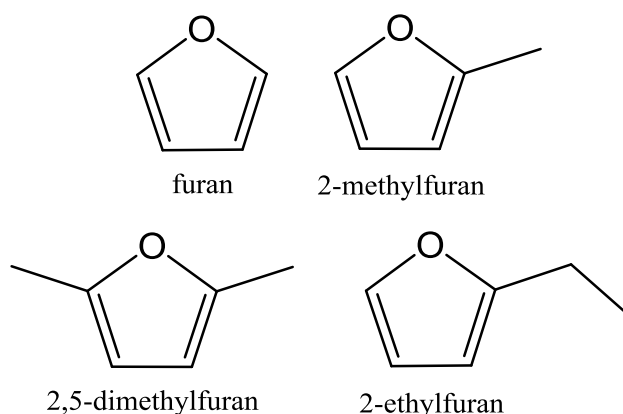
# Kinetics of OH radical reactions with furan and furan derivatives

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Furans are a class of cyclic ethers with promising potential for use as biofuels(1), particularly 2,5-dimethylfuran which has a similar energy density to gasoline.(2) Produced from waste biomass, furans do not come into competition with food crops and therefore do not threaten global food security. Knowledge of the kinetics and mechanisms of the oxidation chemistry of furans will improve the predictive capabilities of combustion mechanisms to aid investigations of their potential use as fuels and the possible impacts of increased use on atmospheric chemistry and composition.



**Figure 1** Derivatives of furan

This work reports the kinetic study of the gas phase reactions of OH with furan derivatives (including furan, 2-methylfuran, 2-ethylfuran and 2,5-dimethylfuran) over a range of temperatures (298-500 K) and pressures (20-95 Torr) by monitoring OH using flash photolysis with laser induced fluorescence (LIF) spectroscopy.

Initial results indicate kinetics to be independent of total pressure and initial conditions, including the presence and concentration of O<sub>2</sub>, with negative temperature dependences observed between 298 and 500 K for furan, 2-methylfuran, 2-ethylfuran and 2,5-dimethylfuran. At 298 K, preliminary results give rate constants of  $(3.27 \pm 0.33) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  for OH + furan,  $(7.67 \pm 0.18) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  for OH + 2-methylfuran,  $(8.84 \pm 0.31) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  for OH + 2-ethylfuran, and  $(12.70 \pm 0.54) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  for OH + 2,5-dimethylfuran.

Relationships between structure, reactivity and mechanism will be discussed with a particular focus on the role of addition reactions.

## References

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