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Technion - Israel Institute of Technology

An open-source toolchain from molecular vibrations to detailed combustion: how (some) physical chemists and chemical engineers have escaped proprietary software

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Citations

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- **Regular (end) citation[1]**
- **Footnote**[1]

[1] Fuller, M. E. et al. Review of Scientific Instruments **2019**, *90*, 064104.

Reaction Classes and Examples

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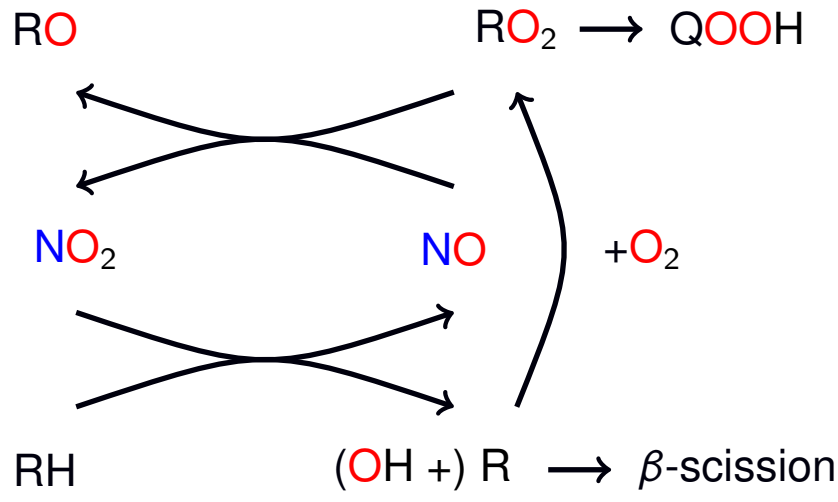
- **Hydrogen abstractions**
  - $RH + NO_2 \rightleftharpoons R + HONO$
  - $RH + NO_2 \rightleftharpoons R + HNO_2$
  - $RH + NO \rightleftharpoons R + HNO$
- **Nitrite/Nitrate/Nitro-/Nitroso-Compounds**
  - $RONO \rightleftharpoons RO + NO$
  - $RONO_2 \rightleftharpoons RO + NO_2$
  - $RNO_2 \rightleftharpoons R + NO_2$
  - $RNO \rightleftharpoons R + NO$
- **Isomerizations**
  - $RONO \rightleftharpoons RNO_2$
- **HONO elimination**
  - $RONO \rightleftharpoons$ alkene + HONO
- **NO_x cycling**
  - $RO_2 + NO \rightleftharpoons RO + NO_2$
  - $R + NO_2 \rightleftharpoons RO + NO$



And when RH is replaced with QOOH or OOQOOH?

Progress on NO_x-Cycling

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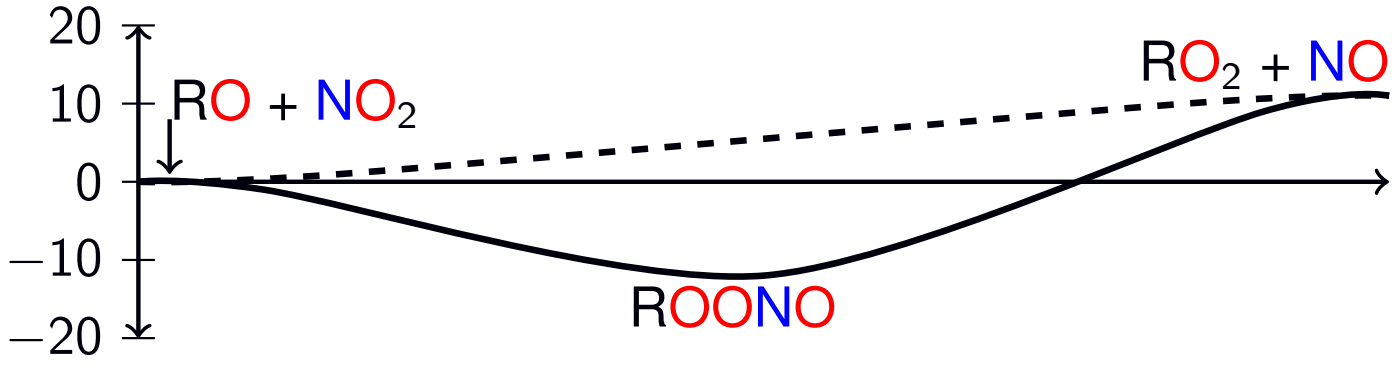

Generalized potential energy surface for alkoxy radical (RO) + NO_2 system. Energies in kcal/mol. Well-skipping occurs at virtually all combustion-relevant temperatures and pressures.

Reaction	A	n	E_a
$CH_3O_2 + NO \rightleftharpoons CH_3O + NO_2$	4.62E+15	-0.38	97.8
$C_2H_5O_2 + NO \rightleftharpoons C_2H_5O + NO_2$	2.11E+14	-0.12	-470.6
$NC_3H_7O_2 + NO \rightleftharpoons NC_3H_7O + NO_2$	1.07E+14	-0.25	-1302.0

Units: centimeters, kelvin, calories, moles

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(1) Fuller, M. E. Energy Conversion and Management **2014**, *88*, 199–205.

(2) Fuller, M. E.; Skowron, M.; Tranter, R. S.; Goldsmith, C. F. Review of Scientific Instruments **2019**, *90*, 064104.

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