

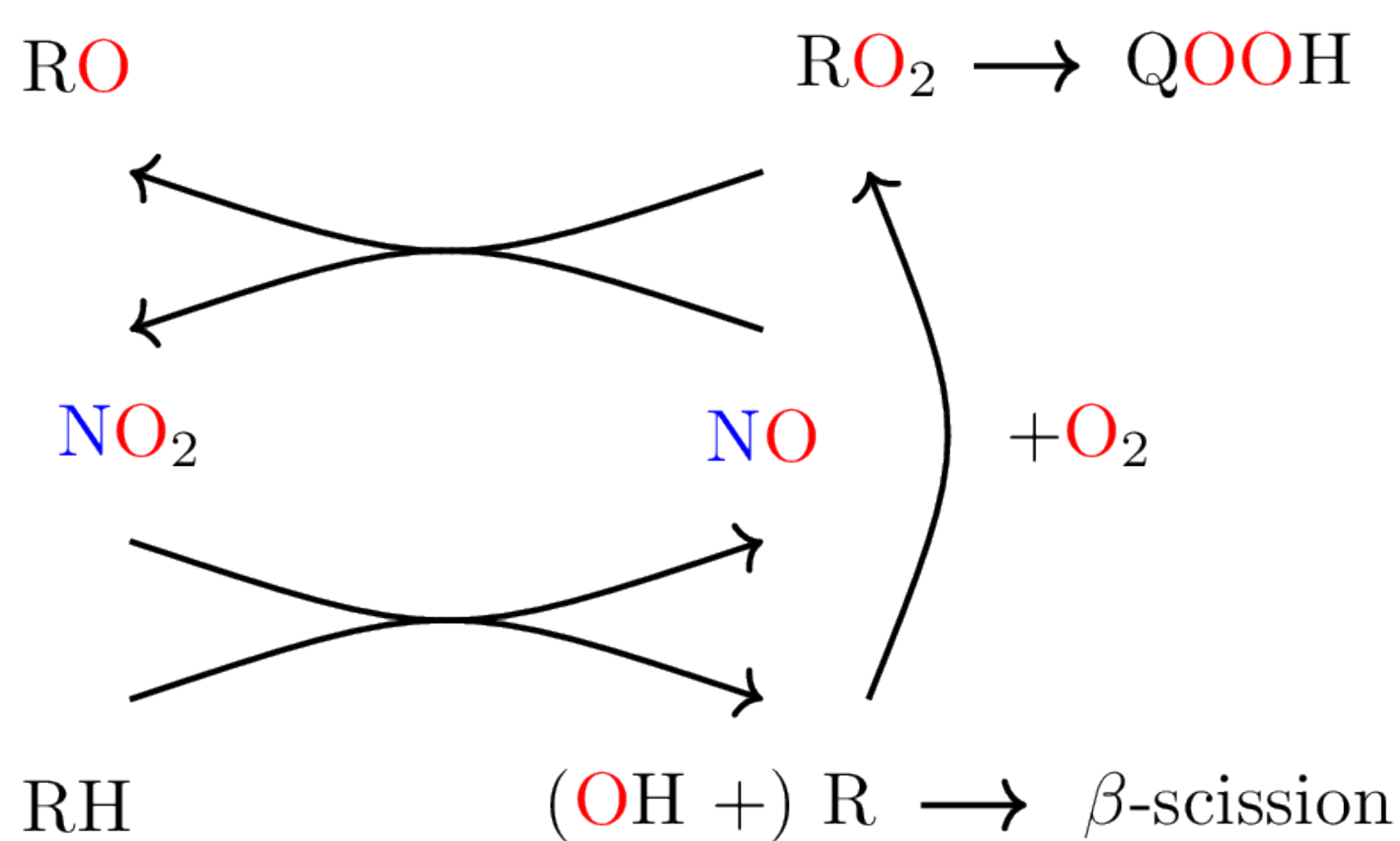
Reaction Class-Based CHON Combustion Mechanism Development

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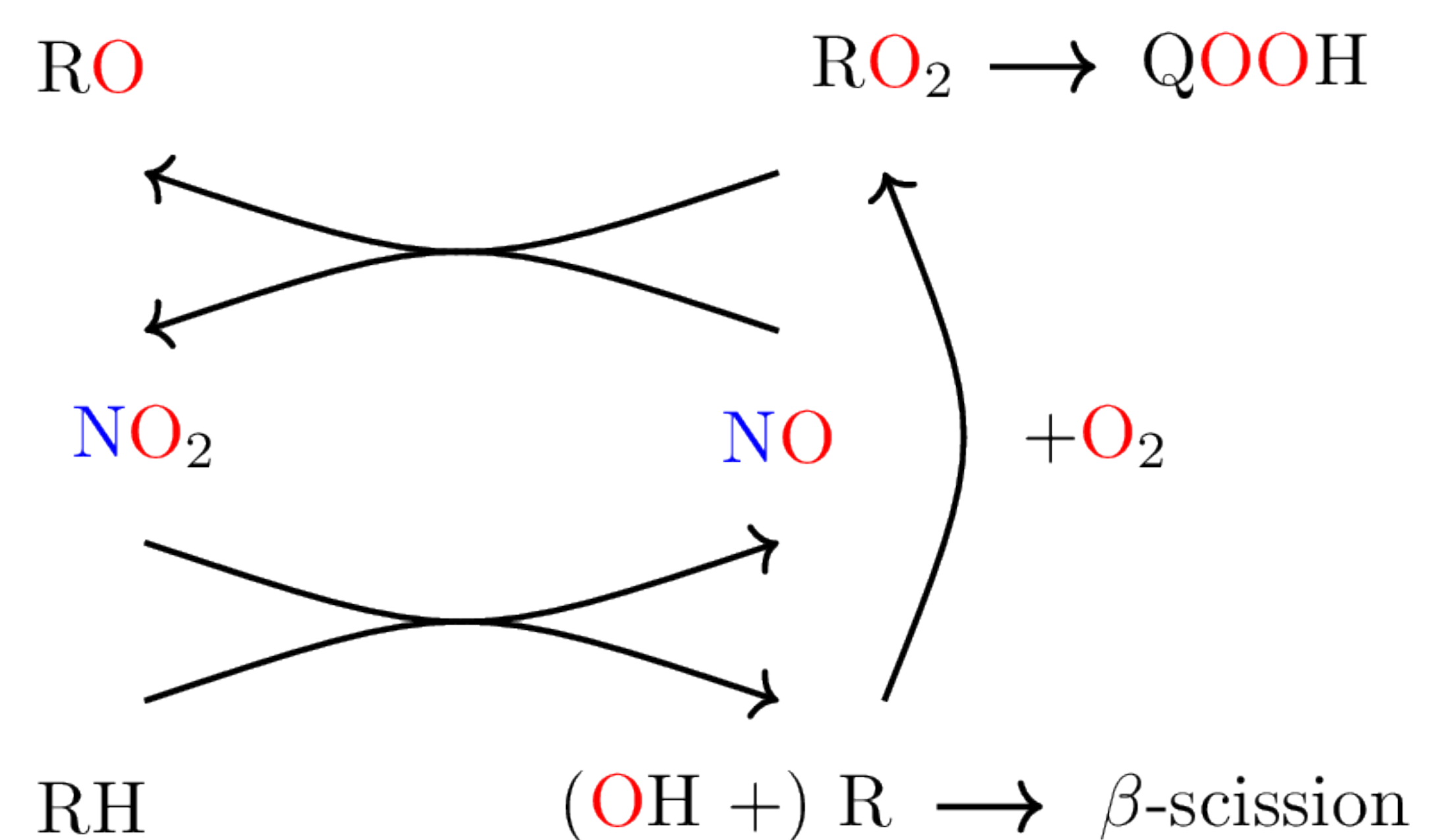
Introduction

- Interactions of NO_x (NO and NO₂) with the combustion process are increasingly relevant in engines with exhaust gas recirculation (EGR) and/or alkyl nitrate cetane enhancers
- Low-temperature combustion reactions with nitrogen are not well-studied and may have significant effects
- Sustainable fuels, produced from bio-based carbon feedstocks, CO₂, and renewable electricity, contain additional functional groups whose reactions with NO_x are not well-characterized

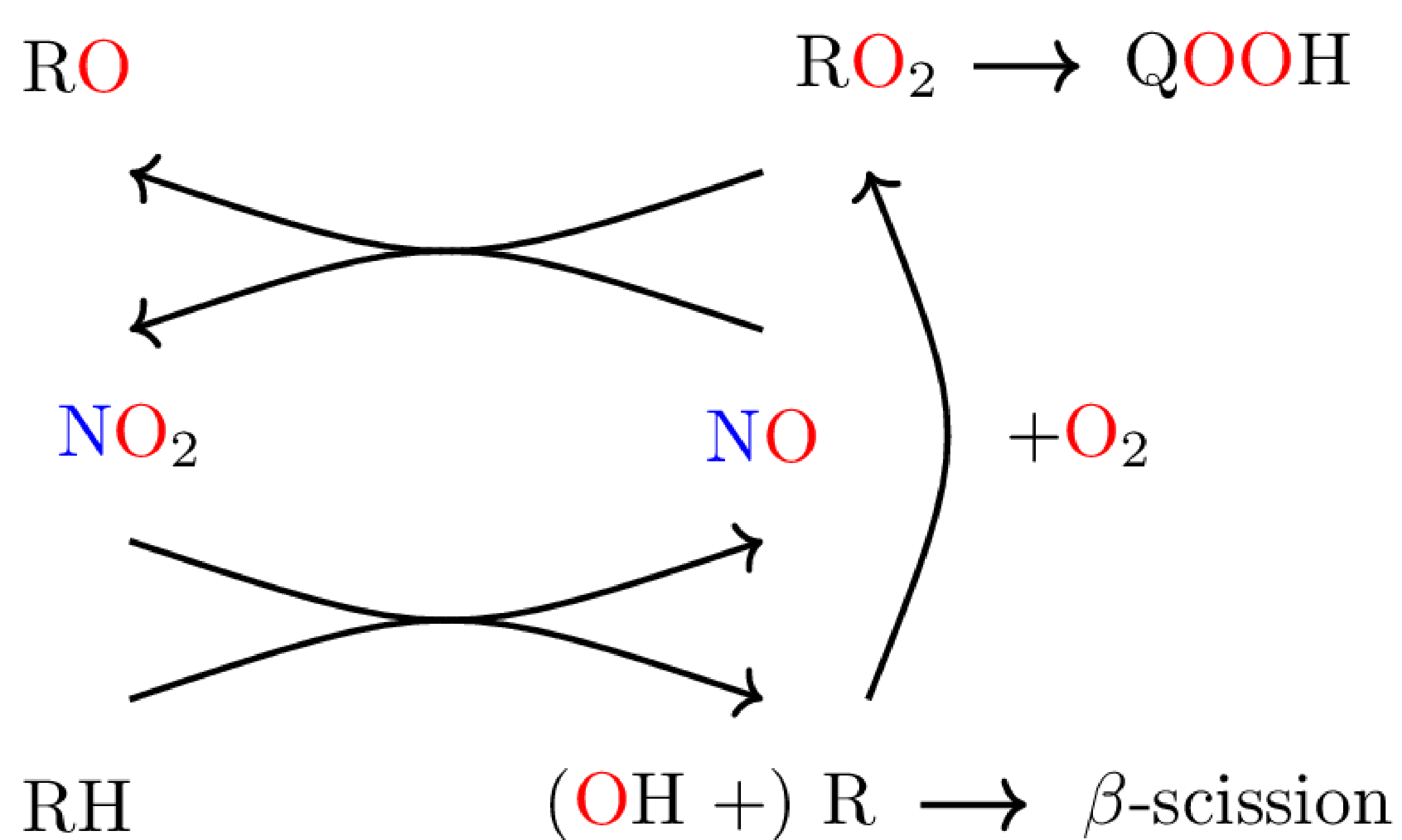


Model Development

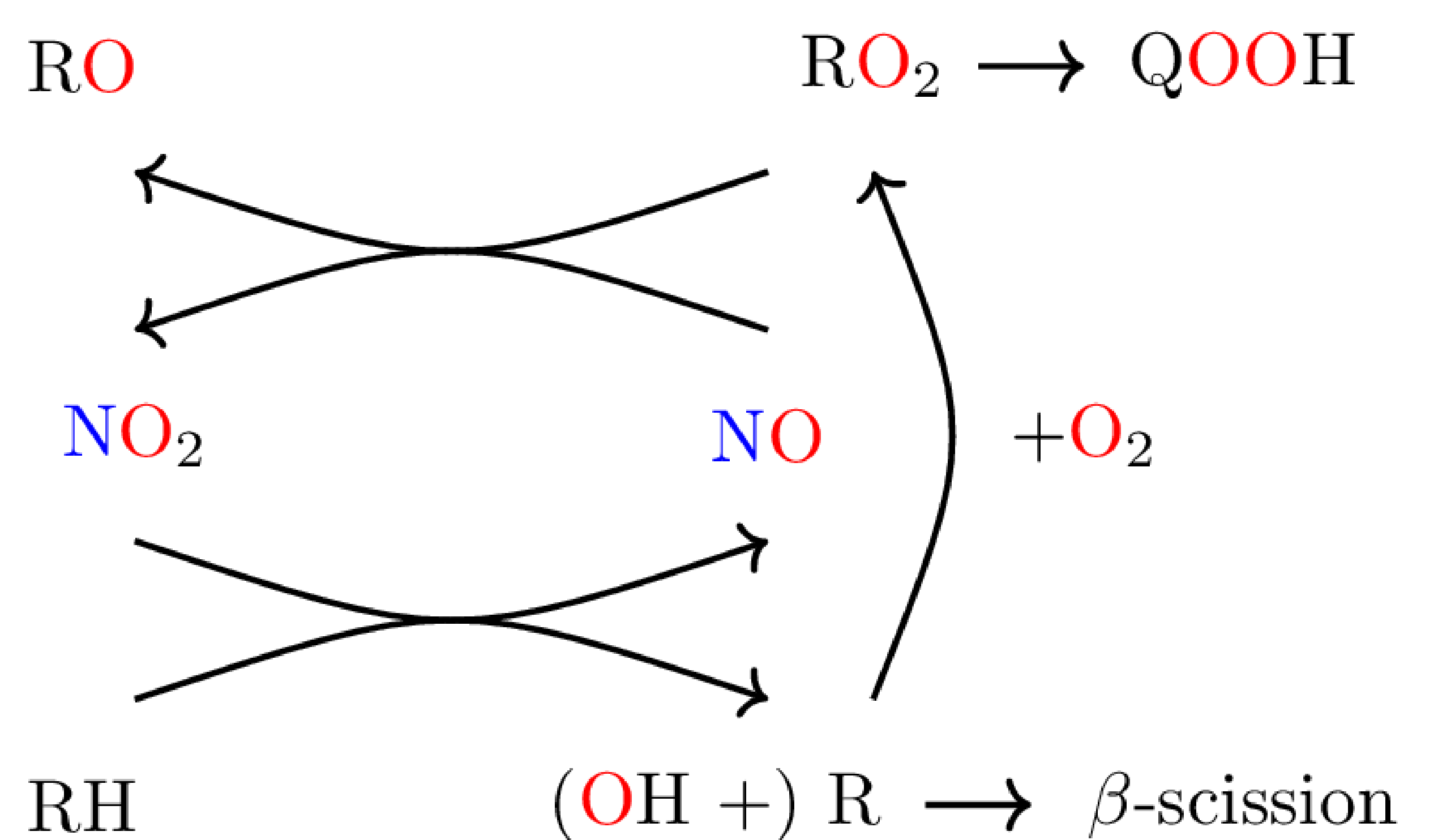
- Pentane isomer mechanism (CHO) of Bugler *et al.* utilized as C₀-C₅ base mechanism



Modeling results



WOW!



Check this shit out!

Work-in-progress

Ab initio calculations

REFERENCES

- M. E. Fuller DOI: 10.1016/j.enconman.2014.08.015.