Supporting information

for

Knowledge-driven design of boron-based catalysts in oxidative dehydrogenation of propane

Weixi Chen, Ziyi Liu, Lihan Zhu, Dongqi Wang*

State Key Laboratory of Fine Chemicals, Liaoning Key Laboratory for Catalytic Conversion of Carbon Resources, School of Chemistry, Dalian University of Technology, Dalian 116024, China

*E-mail: wangdq@dlut.edu.cn (D.W.)

Table S1 Elementary reactions involved in ODHP[1]

step	Reactions
1	$B + O_2 \leftrightarrow BOO\cdot$
2	$C_3H_8 + BOO\cdot \rightarrow \cdot C_3H_7 + B + HOO\cdot$
3	$C_3H_8 + HOO\cdot \rightarrow \cdot C_3H_7 + H_2O_2$
4	$\cdot C_3H_7 + O_2 \rightarrow C_3H_6 + HOO\cdot$
5	$HOO\cdot + * \rightarrow H* + O_2$
6	$H_2O_2 + B \rightarrow *OH + \cdot OH$
7	$C_3H_8 + \cdot OH \rightarrow \cdot C_3H_7 + H_2O$
8	$\cdot OH + * \rightarrow *OH$

Table S2 Equations based on radical chain reaction mechanism of ODH[1]

Equations	order
$\theta_{O2} = \frac{K1PO2\theta B}{K1PO2 + 1}$	1
$\frac{d[\cdot C_3H_7]}{dt} = k_2p_{C3H8}\theta_{O2} + k_3p_{C3H8}[HOO\cdot] - k_4p_{O2}[C_3H_7\cdot] + k_7p_{C3H8}[\cdot OH] = 0$	2
$\frac{d[HOO\cdot]}{dt} = k_2p_{C3H8}\theta_{O2} - k_3p_{C3H8}[HOO\cdot] + k_4p_{O2}[C_3H_7\cdot] - k_5[HOO\cdot]\theta_* = 0$	3
$\frac{d[HO\cdot]}{dt} = k_6[H_2O_2]\,\theta_{B'} - k_7p_{C3H8}[\cdot OH] - k_8[\cdot OH]\theta_* = 0$	4
$\frac{d[H_2O_2]}{dt} = k_3p_{C3H8}[HOO\cdot] - k_6[H_2O_2]\theta_{B'} = 0$	5
$2k_2p_{C3H8}\theta_{O2} - k_5[HOO\cdot]\,\theta_* + k_7p_{C3H8}[\cdot OH] = 0$	6
$k_3p_{C3H8}[HOO\cdot] - k_7p_{C3H8}[\cdot OH] - k_8[\cdot OH]\theta_* = 0$	7

Reference

1. H. Tian, Y. Liu and B. Xu, *Catalysis Today*, 2023, **420**, 114048.