

## Electronic Supplementary Material

### Effect of *cis-/trans* molecular structures on pyrolysis performance and heat sink of decalin isomers

Qing Liu<sup>1,2,4\*</sup>, Kang Xue<sup>1,2,3,4\*</sup>, Tinghao Jia<sup>1</sup>, Zhouyang Shen<sup>1,2,4</sup>, Zehao Han<sup>1,2,4</sup>, Lun Pan  
(✉)<sup>1,2,3,4</sup>, Ji-Jun Zou<sup>1,2,3,4</sup>, Xiangwen Zhang (✉)<sup>1,2,3,4</sup>

1 Key Laboratory for Green Chemical Technology of the Ministry of Education, School of Chemical Engineering and Technology, Tianjin University, Tianjin 300072, China

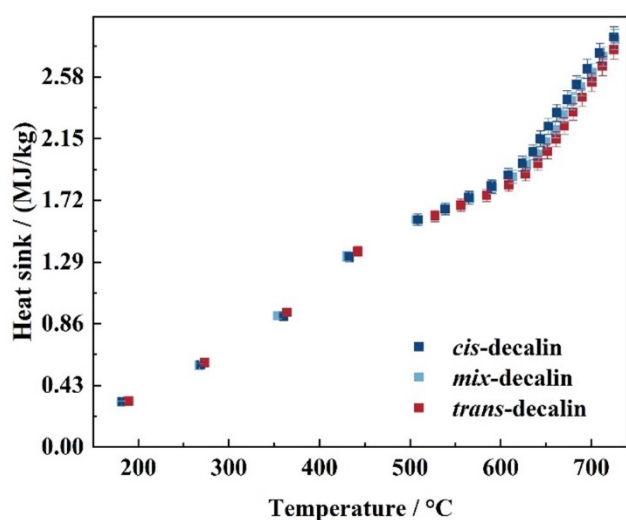
2 Collaborative Innovative Center of Chemical Science and Engineering (Tianjin), Tianjin 300072, China

3 Haihe Laboratory of Sustainable Chemical Transformations, Tianjin 300192, China

4 Zhejiang Institute of Tianjin University, Ningbo 315201, China

\* These authors contributed equally to this work.

E-mails: panlun76@tju.edu.cn (Pan L); zhangxiangwen@tju.edu.cn (Zhang X)



**Fig. S1.** Total heat sink values of pyrolysis of *cis*-, *mix*-, and *trans*-decalin.

**Table S1.** Comparison for the pyrolysis process of the decalin fuels under different conditions in flow reactors.

Fuel	Reaction condition	Residence time/s	Conversion /%	Gas yield/%	Heat sink/ MJ/kg	Refs.
Decalin ( <i>trans</i> : <i>cis</i> =6:4)	550 °C, 5.0 MPa	82.2	9.94	-	1.63	[1]
Decalin ( <i>trans</i> : <i>cis</i> =6:4)	650 °C, 5.0 MPa	59.8	62.75	-	2.17	[1]
Decalin	590 °C, 3.5 MPa	21.4	28	-	-	[2]
Decalin	700 °C, 3.5 MPa	-	92	35	-	[3]
Decalin	650 °C, 4.0 MPa	-	10	5	2.1	[4]
Decalin ( <i>cis</i> : <i>trans</i> - decalin=1:2)	650 °C, 4.0 MPa	1.4	23.2	5	2.13	This work

## References

1. Zhou Z, Mi Z, Zhang X, Fei D. Study on pyrolysis of endothermic propellant decalin in supercritical state. In: International Autumn Seminar on Propellants. Guilin(CN): Explosives & Pyrotechnics (2003 IASPEP), 2003, 1015-1018
2. Xing Y, Wang Q, Fang W. The analysis of decalin pyrolysis property under supercritical

conditions. *Journal of Zhejiang University (Science Edition)*, 2014, 41 (2): 161-167 (in Chinese)

3. Sun D, Li C, Du Y, Kou L, Zhang J, Li Y, Wang Z, Li J, Feng H, Lu J. Effects of endothermic hydrocarbon fuel composition on the pyrolysis and anti-coking performance under supercritical conditions. *Fuel*, 2019, 239: 659-666

4. Li H, Wang Y, Wang L, Zhang X, Liu G. Pyrolysis and coke deposition of JP-10 with decalin in regenerative cooling channels. *Energy & Fuels*, 2022, 36: 6096-6108