

Electronic Supplementary Material







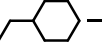
Thermodynamic analysis of reaction pathways and equilibrium yields for catalytic pyrolysis of naphtha

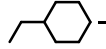




Dongyang Liu, Yibo Zhi, Yuen Bai, Liang Zhao (✉), Jinsen Gao, Chunming Xu

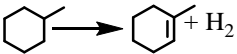
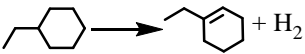
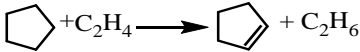
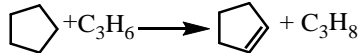
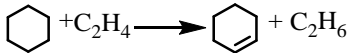
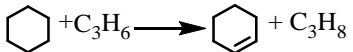
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Table S1 The detailed reaction classes and chemical reactions for C5–8 n/iso/cyclo-paraffins.

Reaction pathway	C5–8 n-paraffins	C5–8 iso-paraffins	C5–8 cyclo-paraffins
Protolytic	$C_5H_{12} \longrightarrow CH_4 + C_4H_8$	$i-C_5H_{12} \longrightarrow CH_4 + i-C_4H_8$	 $\longrightarrow C_2H_4 + C_3H_6$
	$C_5H_{12} \longrightarrow C_2H_6 + C_3H_6$	$i-C_5H_{12} \longrightarrow C_2H_4 + C_3H_8$	 $\longrightarrow 2 C_3H_6$
	$C_5H_{12} \longrightarrow C_3H_8 + C_2H_4$	$i-C_6H_{14} \longrightarrow CH_4 + i-C_5H_{10}$	 $\longrightarrow C_2H_4 + C_3H_6$
	$C_6H_{14} \longrightarrow CH_4 + C_5H_{10}$	$i-C_6H_{14} \longrightarrow C_2H_6 + i-C_4H_8$	 $\longrightarrow C_3H_6 + C_4H_8$
	$C_6H_{14} \longrightarrow C_2H_6 + C_4H_8$	$i-C_6H_{14} \longrightarrow C_3H_6 + C_3H_8$	 $\longrightarrow C_2H_4 + C_5H_{10}$
	$C_6H_{14} \longrightarrow C_3H_8 + C_3H_6$	$i-C_6H_{14} \longrightarrow C_2H_4 + i-C_4H_{10}$	 $\longrightarrow 2 C_4H_8$
	$C_6H_{14} \longrightarrow C_4H_{10} + C_2H_4$	$i-C_7H_{16} \longrightarrow CH_4 + i-C_6H_{12}$	 $\longrightarrow C_3H_6 + C_5H_{10}$

	$C_7H_{16} \longrightarrow CH_4 + C_6H_{12}$	$i-C_7H_{16} \longrightarrow C_2H_6 + i-C_5H_{10}$	 $\longrightarrow C_2H_4 + C_6H_{12}$
	$C_7H_{16} \longrightarrow C_2H_6 + C_5H_{10}$	$i-C_7H_{16} \longrightarrow C_3H_8 + i-C_4H_8$	
	$C_7H_{16} \longrightarrow C_3H_8 + C_4H_8$	$i-C_7H_{16} \longrightarrow C_2H_4 + i-C_5H_{12}$	
	$C_7H_{16} \longrightarrow C_4H_{10} + C_3H_6$	$i-C_7H_{16} \longrightarrow C_3H_6 + i-C_4H_8$	
	$C_7H_{16} \longrightarrow C_5H_{12} + C_2H_4$	$i-C_7H_{16} \longrightarrow C_4H_8 + C_3H_8$	
	$C_8H_{18} \longrightarrow CH_4 + C_7H_{14}$	$i-C_8H_{18} \longrightarrow CH_4 + i-C_7H_{14}$	
	$C_8H_{18} \longrightarrow C_2H_6 + C_6H_{12}$	$i-C_8H_{18} \longrightarrow C_2H_6 + i-C_6H_{12}$	
	$C_8H_{18} \longrightarrow C_3H_8 + C_5H_{10}$	$i-C_8H_{18} \longrightarrow C_3H_8 + i-C_5H_{10}$	
	$C_8H_{18} \longrightarrow C_4H_{10} + C_4H_8$	$i-C_8H_{18} \longrightarrow C_4H_{10} + i-C_4H_8$	
	$C_8H_{18} \longrightarrow C_5H_{12} + C_3H_6$	$i-C_8H_{18} \longrightarrow C_2H_4 + i-C_4H_{10}$	
	$C_8H_{18} \longrightarrow C_6H_{14} + C_2H_4$	$i-C_8H_{18} \longrightarrow C_3H_6 + i-C_5H_{12}$	
		$i-C_8H_{18} \longrightarrow C_2H_4 + i-C_6H_{14}$	
Dehydrogenation	$C_5H_{12} \longrightarrow H_2 + C_5H_{10}$	$i-C_5H_{12} \longrightarrow H_2 + i-C_5H_{10}$	 \longrightarrow  $+ H_2$
	$C_6H_{14} \longrightarrow H_2 + C_6H_{12}$	$i-C_6H_{14} \longrightarrow H_2 + i-C_6H_{12}$	 \longrightarrow  $+ H_2$

	$C_7H_{16} \longrightarrow H_2 + C_7H_{14}$	$i-C_7H_{16} \longrightarrow H_2 + i-C_7H_{14}$	
	$C_8H_{18} \longrightarrow H_2 + C_8H_{16}$	$i-C_8H_{18} \longrightarrow H_2 + i-C_8H_{16}$	
Hydride transfer	$C_5H_{12} + C_2H_4 \longrightarrow C_5H_{10} + C_2H_6$	$i-C_5H_{12} + C_2H_4 \longrightarrow i-C_5H_{10} + C_2H_6$	
	$C_5H_{12} + C_3H_6 \longrightarrow C_5H_{10} + C_3H_8$	$i-C_5H_{12} + C_3H_6 \longrightarrow i-C_5H_{10} + C_3H_8$	
	$C_6H_{14} + C_2H_4 \longrightarrow C_6H_{12} + C_2H_6$	$i-C_6H_{14} + C_2H_4 \longrightarrow i-C_6H_{12} + C_2H_6$	
	$C_6H_{14} + C_3H_6 \longrightarrow C_6H_{12} + C_3H_8$	$i-C_6H_{14} + C_3H_6 \longrightarrow i-C_6H_{12} + C_3H_8$	
	$C_7H_{16} + C_2H_4 \longrightarrow C_7H_{14} + C_2H_6$	$i-C_7H_{16} + C_2H_4 \longrightarrow i-C_7H_{14} + C_2H_6$	
	$C_7H_{16} + C_3H_6 \longrightarrow C_7H_{14} + C_3H_8$	$i-C_7H_{16} + C_3H_6 \longrightarrow i-C_7H_{14} + C_3H_8$	
	$C_8H_{18} + C_2H_4 \longrightarrow C_8H_{16} + C_2H_6$	$i-C_8H_{18} + C_2H_4 \longrightarrow i-C_8H_{16} + C_2H_6$	
	$C_8H_{18} + C_3H_6 \longrightarrow C_8H_{16} + C_3H_8$	$i-C_8H_{18} + C_3H_6 \longrightarrow i-C_8H_{16} + C_3H_8$	
Hydrogen transfer			
			
			
			

			$\text{C}_6\text{H}_{10} + \text{C}_2\text{H}_4 \longrightarrow \text{C}_6\text{H}_8 + \text{C}_2\text{H}_6$
			$\text{C}_6\text{H}_{10} + \text{C}_3\text{H}_6 \longrightarrow \text{C}_6\text{H}_8 + \text{C}_3\text{H}_8$
			$\text{C}_6\text{H}_{11} + \text{C}_2\text{H}_4 \longrightarrow \text{C}_6\text{H}_9 + \text{C}_2\text{H}_6$
			$\text{C}_6\text{H}_{11} + \text{C}_3\text{H}_6 \longrightarrow \text{C}_6\text{H}_9 + \text{C}_3\text{H}_8$