Electronic Supplementary Material (ESI) for Catalysis Science & Technology.

The Partial Oxidation of Propane under Mild Aqueous Conditions with H_2O_2 and ZSM-5 Catalysts. Supporting Information

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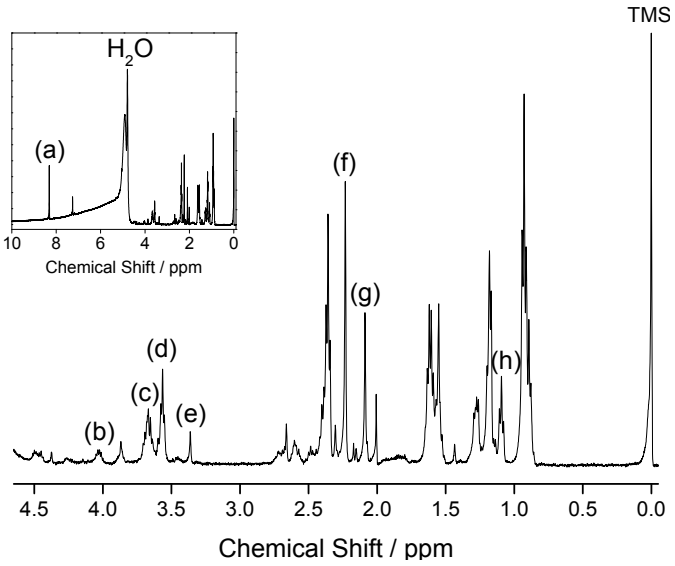

Assignment (Chemical Shift δ / ppm)	Product	Protons
a (8.31)	Formic Acid	**H**COOH
b (4.02)	Isopropanol	$(CH_3)_2C\mathbf{H}OH$
c (3.65)	Ethanol	$CH_3C\mathbf{H}_2OH$
d (3.55)	n-Propanol	$CH_3CH_2C\mathbf{H}_2OH$
e (3.37)	Methanol	$C\mathbf{H}_3OH$
f (2.23)	Acetone	$(C\mathbf{H}_3)_2CO$
g (2.07)	Acetic Acid	$C\mathbf{H}_3COOH$
h (1.09)	Propanoic Acid	$C\mathbf{H}_3CH_2COOH$

Figure S1 A typical solvent- suppressed ^{1}H-NMR spectrum for propane oxidation reactions, with assignment of resonances used in product quantification.

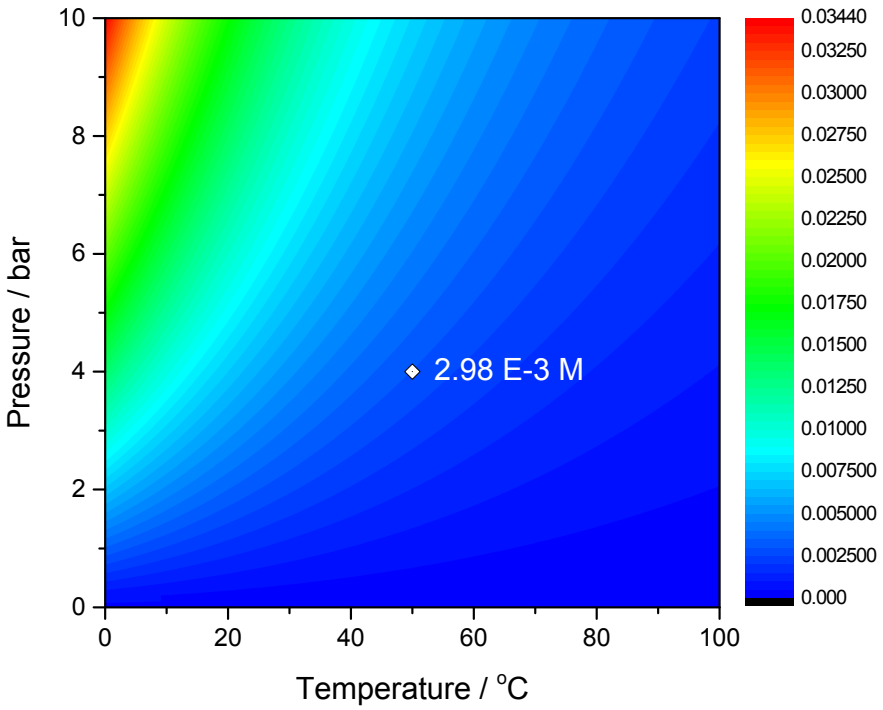

Figure S2 The solubility of propane in water as a function of $P(C_3H_8)$ and temperature as calculated using Henry's Law. ❋ Propane solubility under standard conditions $P(C_3H_8)$ = 4 bar and 50 °C.

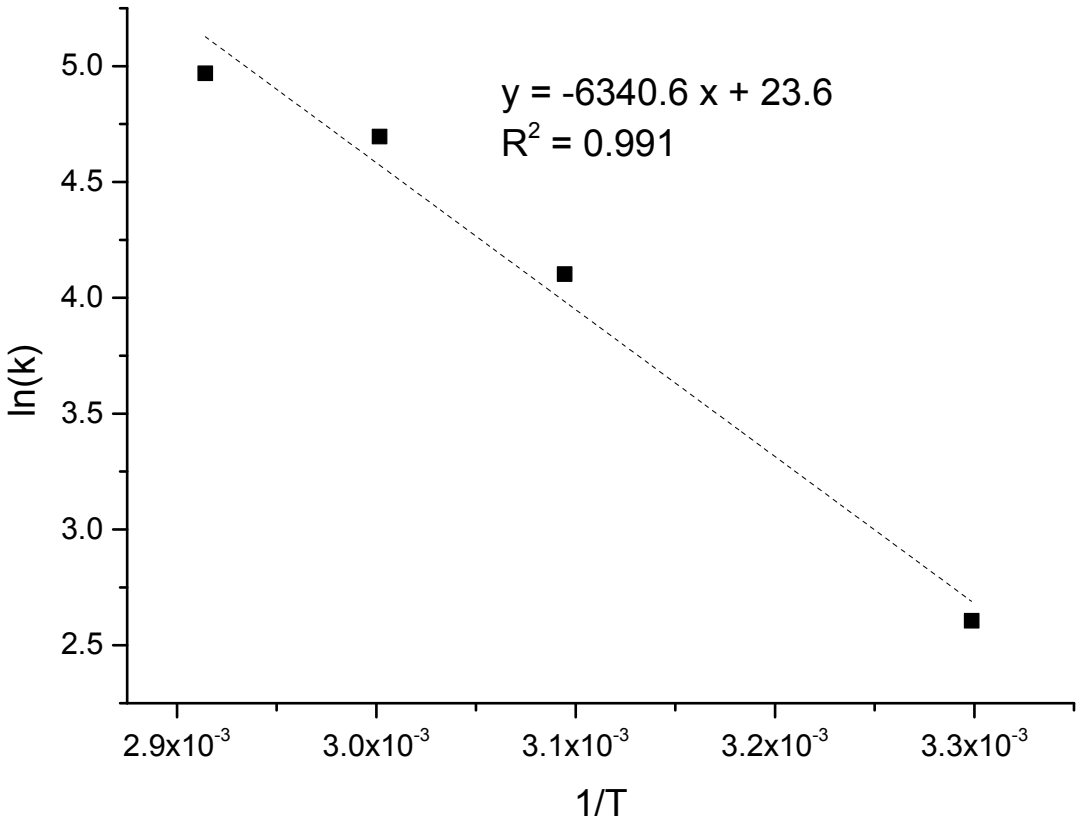

Figure S3 Arrhenius plot for data in Figure 8

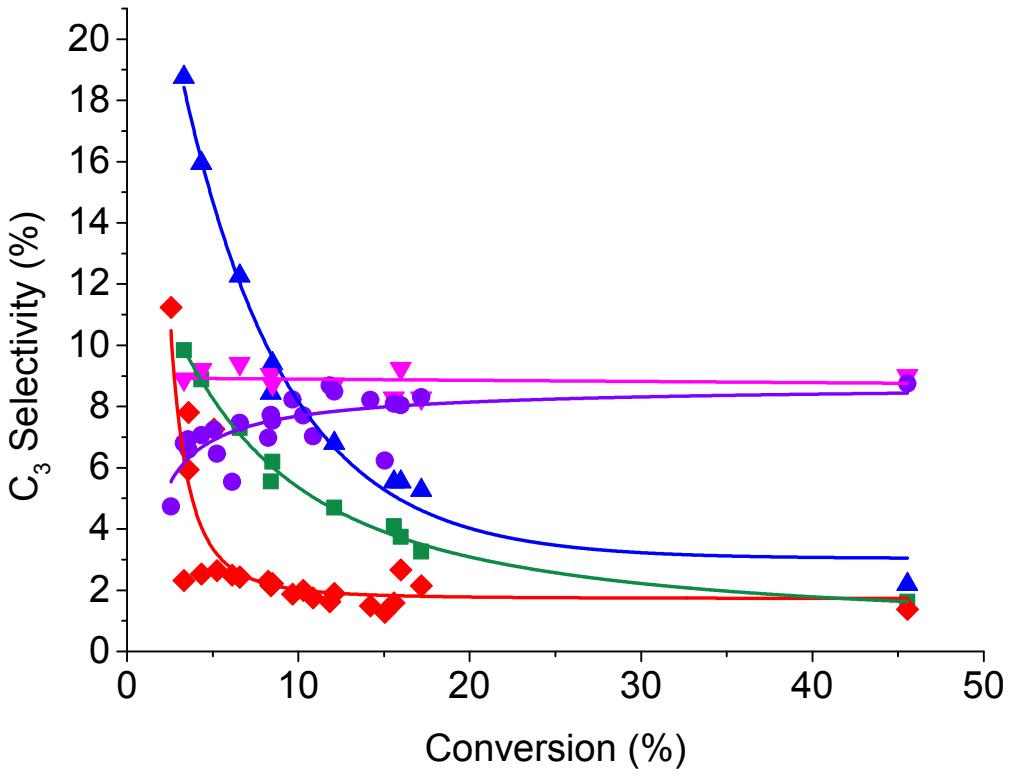

Figure S4 – Effect of conversion on C3 products selectivity. n-Propanol (□), isopropanol (■), acetone (●), propene (♦) and propanoic acid (❑)

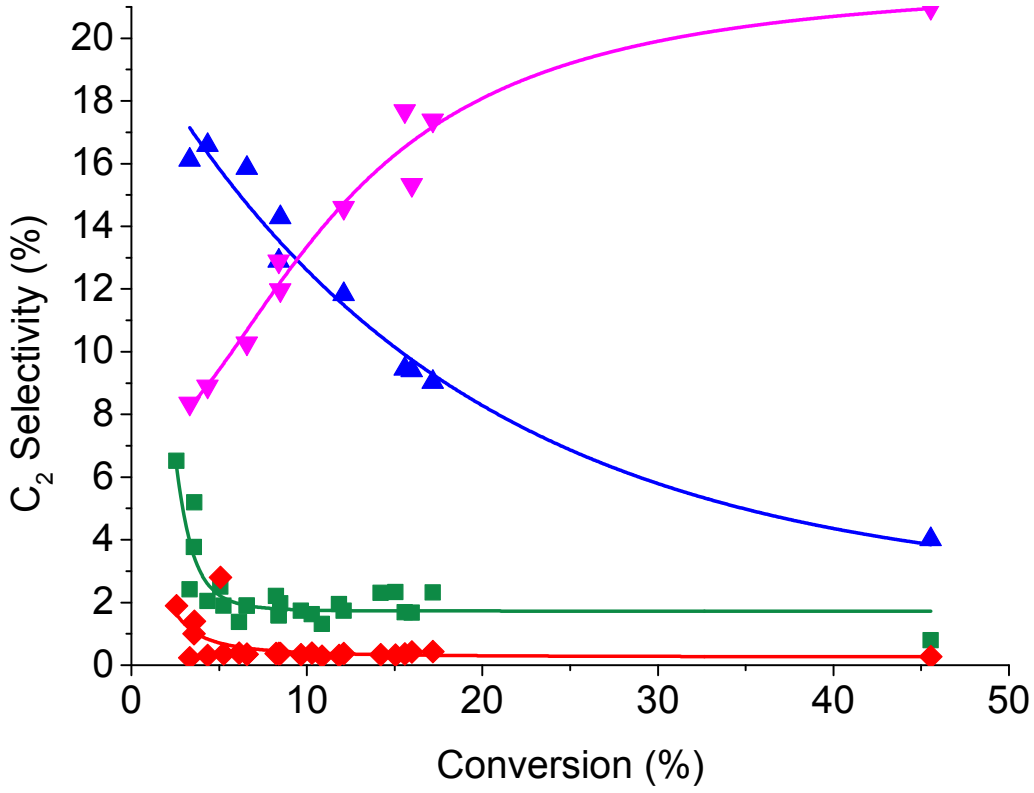

Figure S5 – Effect of conversion on C2 products selectivity. Ethanol (□), Ethane (■), Ethene (♦) and Acetic acid (❑)

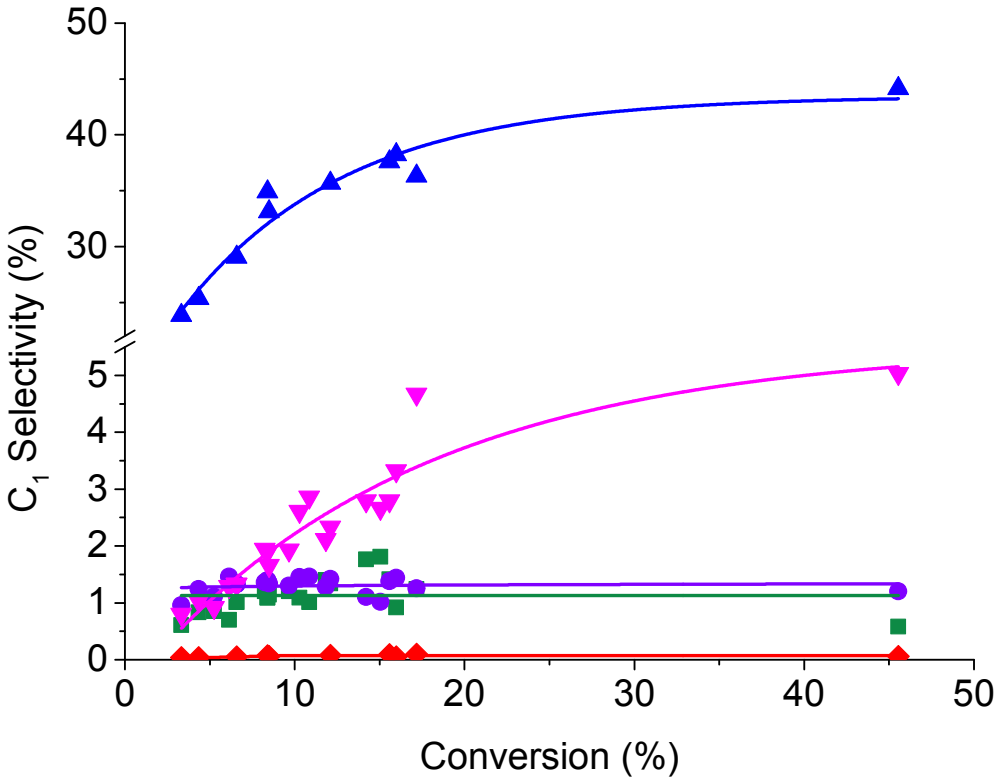

Figure S6 – Effect of conversion on C1 products selectivity. Formic acid (□), methane (■), methanol (●), CO (♦) and CO_2 (❑)

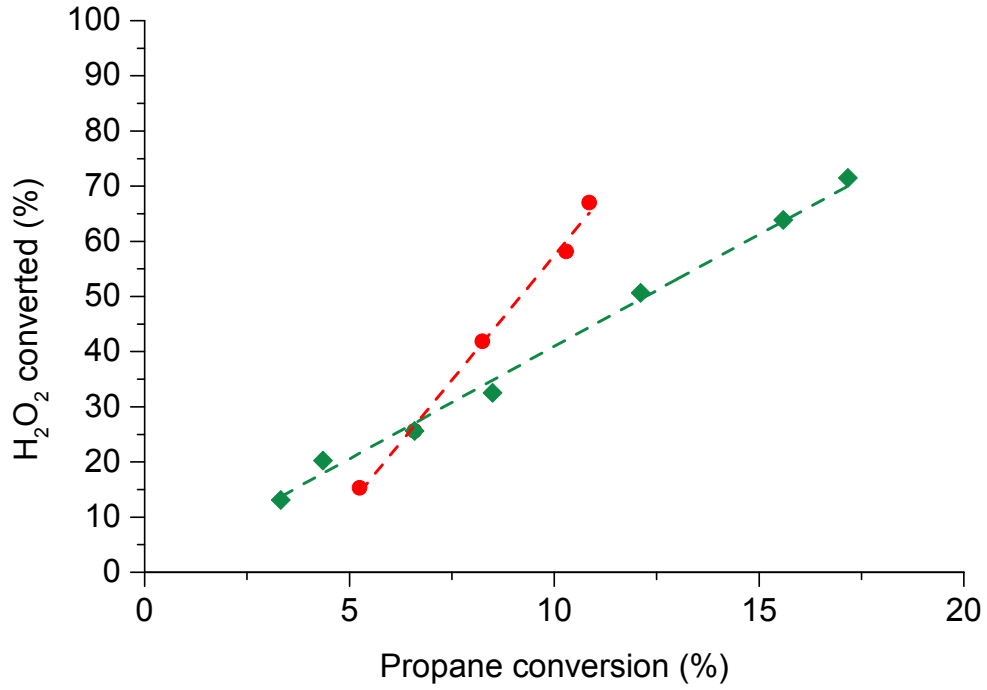

Figure S7 – Effect of conversion on H_2O_2 conversion. Catalyst mass study (●), reaction time study

Table S1 A comparison of the catalytic performance of H-ZSM-5 (30) and 2.5 % Cu/ZSM-5 (30) (CVI) under standard propane oxidation reaction conditions.

Catalyst	Propane conversion / %	H_2O_2 Conversion / %	Product Selectivities / %												
			C3 Products				C_2 Products					C_1 Products			
			Acetone	*i*-PrOH	*n*-PrOH	Propanoic Acid	C_3H_6	EtOH	Acetic Acid	C_2H_4	C_2H_6	MeOH	Formic Acid	CH_4	CO_2
H-ZSM-5 (30)	0.90	5.0	7.6	8.4	18.2	11.7	2.5	7.7	6.2	0.4	6.1	0.9	28.1	1.3	0.8
2.5 % Cu/ZSM-5 (30)	0.36	5.4	9.3	19.8	18.8	3.2	20.8	1.4	1.0	2.1	12.6	2.5	4.0	3.2	1.2

Reaction conditions for Entry 1: Propane (4000 μmol), $[H_2O_2]$ = 0.5 M (5000 μmol), 27 mg catalyst, 50 ºC, 0.5 h, 1500 rpm.