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APPENDICES

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APPENDIX A

CALULATION OF CATALYSY PREPARATION

Calculation of the preparation of zinc gallate and zinc aluminate.

In this study zinc gallate and zinc aluminate were prepared in each organic solvent have 4 different charged of Zn/Ga or Zn/Al atomic ratios, Zn/Ga or Zn/Al = 0.25, 0.33, 0.50 and 1.00

Zinc acetate and gallium acetylacetone are used as the reactants for the synthesis of zinc gallate. For the preparing of zinc gallate powder.

1. Gallium acetylacetone ($\text{Ga}(\text{acac})_3$, $[\text{CH}_3\text{COCH}=\text{C}(\text{O}-)\text{CH}_3]_3\text{Ga}$) has molecular weight (M.W) of 367.05 g/mol.

Gallium (Ga) has M.W. of 69.72 g/mol.

2. Zinc acetate ($(\text{CH}_3\text{COO})_2\text{Zn}$) has M.W. of 183.46 g/mol.

Zinc (Zn) has M.W. of 65.37

Gallium acetylacetone 5 g used for preparation of zinc all Zn/Ga atomic ratios.

The reagents 5 g were equal to:

$$\text{Gallium} = (69.72/367.05) \times 5 = 0.9497 \text{ g} = 0.0136 \text{ mol}$$

Zinc equal to:

$$\text{Zinc} = 0.5 \times 0.0136 = 0.0068 \text{ mol} = 0.4452 \text{ g}$$

From zinc 0.4452 g, zinc acetate is used equal to:

$$\text{So, weight of zinc acetate} = (183.46/65.37) \times 0.4452 \text{ g} = 1.2496 \text{ g}$$

The results of calculation of all Zn/Ga atomic ratios are shown in table A1.

Table A.1 Reagent used for the synthesis of zinc gallate.

Zn/Ga atomic ratio	Gallium acetylacetonate	Zinc acetate
0.25	5 g	0.6806 g
0.33	5 g	0.8330 g
0.50	5 g	1.2496 g
1.00	5 g	2.4991 g

Similarly, the calculation of the preparation of the zinc aluminate is shown as follow:

Zinc acetate and aluminium isopropoxide (AIP) are use as the reactants for the preparing zinc aluminate powder.

1. Aluminium isopropoxide (AIP, $[(\text{CH}_3)_2\text{CHO}]_3\text{AL}$) has M.W. of 204.25 g/mol.
Aluminium has M.W. of 26.98 g/mol.
2. Zinc acetate $((\text{CH}_3\text{COO})_2\text{Zn}$) has M.W. of 183.46 g/mol
Zinc (Zn) has M.W. of 65.37

Aluminium isopropoxide 5 g were used for preparation of all Zn/Al atomic ratio.

The reagent 5 g were consisted of aluminium isopropoxide more than:

$$\text{Aluminium isopropoxide} = (98/100) \times 5 = 4.90 \text{ g.}$$

So, aluminium isopropoxide 4.90 g were consisted of aluminium equal to:

$$\text{Aluminium} = (26.98/204.25) \times 4.90 \text{ g} = 0.6604 \text{ g} = 0.0245 \text{ mol}$$

So, Zn/Al = 0.5 has zinc equal to:

$$\text{Zinc} = 0.5 \times 0.0245 = 0.0122 \text{ mol} = 0.7975 \text{ g}$$

From zinc 0.7975 g , zinc acetate is used equal to:

$$\text{So, weight of zinc acetate} = (183.46/65.37) \times 0.7975 \text{ g} = 2.2404 \text{ g}$$

The results of calculation of all Zn/Al atomic ratios are shown in Table A2.

Table A.2 Reagent use for the synthesis of zinc aluminate.

Zn/Al atomics ratio	Aluminium isopropoxide	Zinc acetate
0.33	5 g	1.4670 g
0.50	5 g	2.2404 g
1.00	5 g	4.4012 g

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APPENDIX B

CALCULATION OF REACTANT FLOW RATE

B1. Calculation of the flow rate of C₃H₈, air and helium in the ratio of 4:8:88

The sample of calculation shown below is for feed composition of 4 vol. % propane, 8 vol. % oxygen and balance helium.

Total flow rate = 100 ml/min.

Flow rate of 21% O₂ in air is assumed to be X ml/min

Flow rate of 20% C₃H₈ in helium is assumed to be Y ml/min

If feed flow rate contains 8% oxygen,

Then there is O₂ in flow of O₂; $21X/100 = 8$

Also there is C₃H₈ in flow of C₃H₈ in He; $20Y/100 = 4$

There for $X = 38.09 \text{ ml/min}$

$Y = 20 \text{ ml/min}$

Argon is used as balance gas, hence its flow is equal to $100 - 38.09 - 20$

$$= 41.91 \text{ ml/min}$$

B2. Calculation of checking explosive limit of propane in air.

The explosive limit of propane in air is shown below:

	Lower limit in air	Upper limit in air
propane	2.37 %	9.5%

Therefore, the amount of propane in feed must not be in the range of this explosive limit (between 2.37 – 9.5 % in air)

Calculation for the condition of feed stream 4:8:88

Flow rate C₃H₈ used in this study is fixed to 4 ml/min.

Flow rate of air is 38.09 ml/min

$$\begin{aligned}\text{Hence, there are propane in air} &= (4/38.09) \times 100 \\ &= 10.50\% \end{aligned}$$

APPENDIX C

SUMMARY OF EXPERIMENT RESULTS

Data of catalyst reaction

Table C.1 Reaction data of zinc gallate (atomic ratio 1.00,) for figure 5.3, 5.4, and 5.5

Temperature (°C)	Propane conversion	Propylene selectivity	Propylene yield
400	5.75	13.35	0.76
450	5.27	16.86	0.88
500	22.82	7.92	1.8
550	65.12	3.58	2.35
600	60.01	4.9	2.94

Table C.2 Reaction data of zinc gallate (atomic ratio 0.50) for figure 5.3, 5.4, and 5.5.

Temperature (°C)	Propane conversion	Propylene selectivity	Propylene yield
400	3.08	26.36	0.81
450	2.5	41.74	1.04
500	48.41	6.33	3.07
550	65.14	17.46	11.38
600	66.4	20.02	13.29

Table C.3 Reaction data of zinc gallate (atomic ratio 0.33) for figure 5.3, 5.4, and 5.5.

Temperature (°C)	Propane conversion	Propylene selectivity	Propylene yield
400	5.72	82.65	4.73
450	12.05	52.69	6.34
500	36.35	18.08	6.57
550	49.25	12.56	6.18
600	38.22	11.52	4.4

Table C.4 Reaction data of zinc gallate (atomic ratio 0.25) for figure 5.3, 5.4, 5.5.

Temperature (°C)	Propane conversion	Propylene selectivity	Propylene yield
400	3.22	70.42	5.49
450	7.7	47.58	3.66
500	49.42	14.65	7.24
550	56.97	13.35	7.6
600	65.94	11.37	7.5

Table C.5 Reaction data of zinc aluminate (atomic ratio 1.00) for figure 5.6, 5.7, 5.8.

Temperature (°C)	Propane conversion	Propylene selectivity	Propylene yield
400	7.5	60.27	4.75
450	11.9	38.5	4.6
500	20.1	23.82	4.78
550	28.02	18.28	5.12
600	52.88	10.55	5.57

Table C.6 Reaction data of zinc aluminate (atomic ratio 0.50) for figure 5.6, 5.7, 5.8.

Temperature (°C)	Propane conversion	Propylene selectivity	Propylene yield
400	0.40	91.5	0.36
450	5.84	85.52	4.8
500	8.37	59.5	5.21
550	11.05	58.96	6.51
600	30.73	23.93	7.35

Table C.7 Reaction data of zinc aluminate (atomic ratio 0.33) for figure 5.6, 5.7, 5.8.

Temperature (°C)	Propane conversion	Propylene selectivity	Propylene yield
400	3.45	68.67	3.45
450	9.27	55.58	5.15
500	10.5	46.13	4.48
550	16.34	41.46	6.77
600	38.65	20.16	7.79

APPENDIX D

CALCULATION OF BET SURFACE AREA BY THE SINGLE METHOD

From Brunauer-Emmett-Teller (BET) equation:

$$\frac{X}{V(1-X)} = \frac{1}{VmC} + \frac{(C-1)X}{VmC} \quad (C.1)$$

Where: X = relative partial pressure of N_2 , P/P_o

P_o = saturated vapor pressure of N_2 (or adsorbed gas) at the experimental temperature

P = equilibrium vapor pressure of N_2

V = volume of gas adsorbed at a pressure P ; ml at the NTP/ g of sample

V_m = volume of gas adsorbed at monolayer, ml at the NTP/ g of sample

C = constant

Assume $C \rightarrow \infty$, then

$$\frac{X}{V(1-X)} = \frac{X}{Vm} \quad (C.2)$$

$$Vm = V(1 - P/P_o)$$

From the gas law,

$$\frac{P_b V}{273} = \frac{P_t V}{T} \quad (C.3)$$

Where: V = constant volume

P_b = pressure at $0^\circ C$

P_t = pressure at $t^\circ C$

$T = 273.15 + t$, K

$P_t = 1$ atm and thus, $P_b = (273.15/T)$

Partial pressure of Nitrogen:

$$P = \frac{[Flow of (He + N_2) - Flow of He]}{Flow of (He + N_2)} \quad (C.4)$$
$$= 0.3 \text{ atm}$$

N_2 saturated vapor pressure, $P_o = 1.1$ atm

$$p = P/P_o = P/1.1 = 0.3/1.1 = 0.2727$$

How to measure V

$$V = \frac{S_2}{S_1} \times \frac{1}{W} \times \frac{273.15}{T} \text{ ml./ g of catalyst} \quad (C.5)$$

Where: S_1 = Nitrogen 1 ml/ 1 atm of room temperature area

S_2 = Desorption of nitrogen area

W = Weight of the sample (g)

T = Room temperature (K)

Therefore,

$$\begin{aligned} V_m &= \frac{S_2}{S_1} \times \frac{1}{W} \times \frac{273.15}{T} \times (1-p) \\ V_m &= \frac{S_2}{S_1} \times \frac{1}{W} \times \frac{273.15}{T} \times 0.7273 \end{aligned} \quad (C.6)$$

Surface area of catalyst:

$$S = \frac{N\sigma V_m}{M}$$

Where: N = Avogadro number = 6.02×10^{23}

σ = area occupied by one molecule of adsorbed nitrogen = 16.2×10^{-20}

M = volume of one mole nitrogen = $22410 \text{ cm}^3/\text{mol}$

Then,

$$\begin{aligned} S &= 4.352 V_m \\ S &= \frac{S_2}{S_1} \times \frac{1}{W} \times \frac{273.15}{T} \times 0.7273 \times 4.352 \\ S &= \frac{S_2}{S_1} \times \frac{1}{W} \times \frac{273.15}{T} \times 3.1582 \end{aligned} \quad (C.7)$$

APPENDIX E

CALIBRATION CURVES

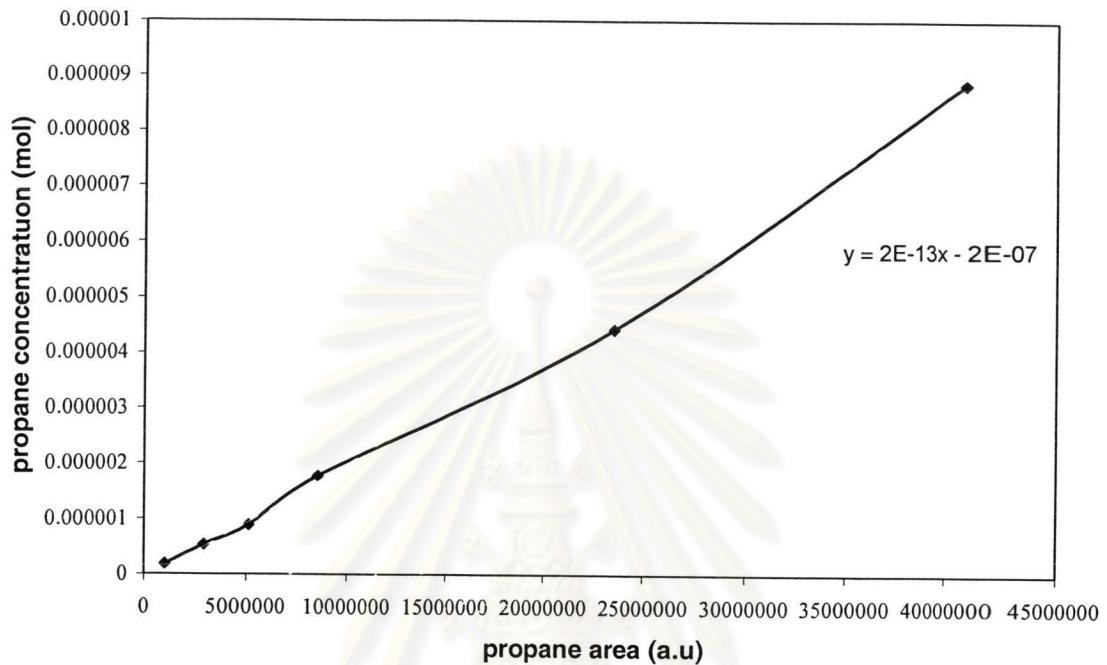


Figure E.1 The calibration curve of propane

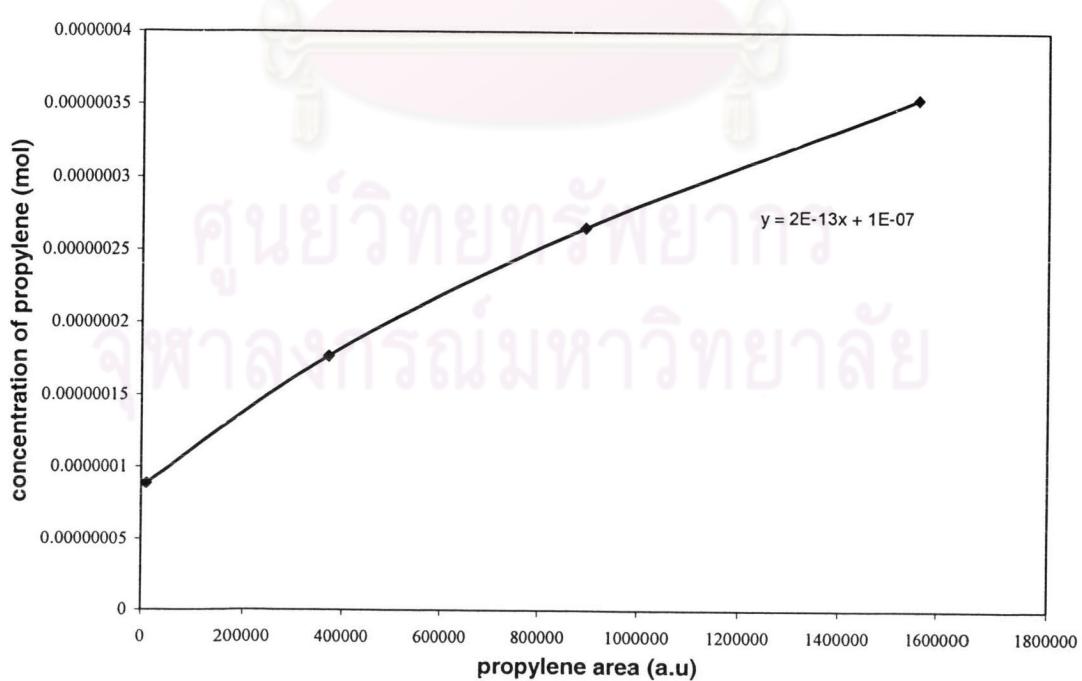


Figure E.2 The calibration curve of propylene

VITA

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