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APPENDICES

APPENDIX

A-1 Physical Property of the Two Commercial Mordenites

	Na-mordenite	H-mordenite
Si/Al mol ratio (in catalog)	9.15	110
Si/Al mol ratio (Analysis results)	11	120
Na_2O (wt.%)	4.5	<0.05
Surface area (BET, m^2/g)	360	420
Crystal size (μm)	0.1 × 0.5	0.1 × 0.5
Mean particle size (μm)	10-12	5-7

B-1 Calculation for Vapor Pressure of Methanol

Antoine's equation

$$\ln (P \times (Vp/P_c)) = (1-X)^{-1}[(VpA)X + (VpB)X^{1.5} + (VpC)X^3 + (VpC)X^6] \qquad (A\text{-}1)$$

Where P = Total pressure

Vp = Vapor pressure

P_c = Critical pressure

$X = 1 - (T/T_c)$; T_c = critical temperature, T = trial temperature (K)

VpA, VpB, VpC, VpD = constant

Example: Determination of vapor pressure of methanol at 29°C

For methanol; $T_c = 512.6$ K, $P_c = 80.9$ atm, $P = 1$ atm

VpA = -8.54796, VpB = 0.76982, VpC = -3.10850,

VpD = 1.54481, T = 29°C = 302.15 K

$X = 1 - (302.15/512.6) = 0.41055$

$$\ln (1\times(Vp/80.9)) = (1-0.41055)^{-1}[(-8.54796)(0.41055) + (0.76982)(0.41055)^{1.5} + (-3.10850)(0.41055)^3 + (1.54481)(0.41055)^6]$$

$\ln (Vp/80.9) = -5.9883$

$Vp/80.9 = \exp(-5.9883) = 2.5079 \times 10^{-3}$

$Vp = 0.2029$ atm

B-2 Calculation for Feed Flow Rate

The used catalyst = 0.4 g

Packed catalyst into borosilicate reactor (inside diameter = 0.54 cm)

Determine the average height of catalyst bed = 2.6 cm, so that,

Volume of bed $= \pi r^2 h = (22/7) \times (0.27)^2 \times 2.6$

$= 0.5957\ cm^3$-cat.

Use Gas Hourly Space Velocity (GHSV) = 2000 h^{-1}

$$GHSV = \frac{\text{Volumetric flow rate}}{\text{Volume of bed}} \quad \text{at STP condition}$$

Volumetric flow rate $= 2000 \times 0.5957 = 1191.40\ cm^3/h$

$= 1191.40/60 = 19.86\ cm^3/min$

At room temperature

$$\text{Volumetric flow rate} = 19.86 \left(\frac{273.15 + T}{273.15}\right),$$

Where T = measured temperature of methanol saturator (°C)

B-3 Calculation for Conversion of Methanol in MTO reaction

Methanol conversion activity was evaluated in term of conversion of methanol into other hydrocarbons.

$$\text{Methanol conversion (\%)} = \frac{(A_{in} - A_{out})}{A_{in}} \times 100 \qquad \text{(A-2)}$$

Where A = GC peak area of methanol

If $A_{in} = 10650$; $A_{out} = 0$

$$\text{Methanol conversion (\%)} = \frac{(10650 - 0)}{10650} \times 100$$

$$= 100\%$$

B-4 Calculation of GC Peak Area to Concentration

$$C_x = \frac{A_x \times C_{std} \times V_{std}}{A_{std} \times V_x} \quad \text{(A-3)}$$

$$\% \text{ selectivity} = \frac{C_x \times 100}{C_{total}} \quad \text{(A-4)}$$

When C_{std} = Concentration of the component of interest in the standard mixture, % mol

C_x = Concentration of the component in the sample, % mol.

C_{total} = Concentration of the total component in the sample, % mol.

A_{std} = Peak area of the component in standard mixture, au.

A_x = Peak area of the component in the sample, au.

V_{std} = injected volume of the standard mixture, μl.

V_x = injected volume of the sample, μl.

If data of proylene, $A_{propylene} = 145462$; $A_{std} = 77006$; $C_{std} = 15.0$ % molar;

$V_{std} = 1.5$ μl; $V_{propylene} = 10$ μl, $C_{total} = 13.13$ % molar

$$C_{propylene} = \frac{145462 \times 15.0 \times 1.5}{77006 \times 10}$$

$$= 4.25\% \text{ molar}$$

$$\% \text{ selectivity to propylene} = \frac{4.25 \times 100}{13.13}$$

$$= 32.37$$

B-5 Calculation for Initial Weight of Feed Methanol

$$P\,V = n\,RT \qquad \text{(A-5)}$$

When P = partial pressure of methanol, atm

V = volumn of gas, L

n = mole of methanol, mol

R = constant = 0.082 atm • L • mol^{-1} • K^{-1}

T = temperature of methanol, K

If P = 0.2029 atm, V = 0.8776 L, T = 29°C = 302.15 K

$$n = \frac{P\,V}{R\,T}$$

$$= \frac{0.2029 \times 0.8776}{0.082 \times 302.15}$$

$$= 0.007187 \text{ mol} = 0.2303 \text{ g}$$

B-6 Calculation for Yield of Gas Product and Liquid Product

$$\% \text{ Yield of liquid product} = \frac{\text{wt. liquid product} \times 100}{\text{wt. MeOH}} \quad \text{(A-6)}$$

$$\% \text{ Yield of gas product} = \frac{\text{wt. gas product} \times 100}{\text{wt. MeOH}} \quad \text{(A-7)}$$

When wt. gas product = wt.MeOH – wt. liquid product – wt. coke

If wt. MeOH = 0.2303 g, wt. liquid product = 0.0925 g, wt. coke = 0.0162 g

$$\% \text{ Yield of liquid product} = \frac{0.0925 \times 100}{0.2303}$$

$$= 40.17$$

$$\% \text{ Yield of gas product} = \frac{0.2303 - 0.0925 - 0.0162 \times 100}{0.2303}$$

$$= 52.80$$

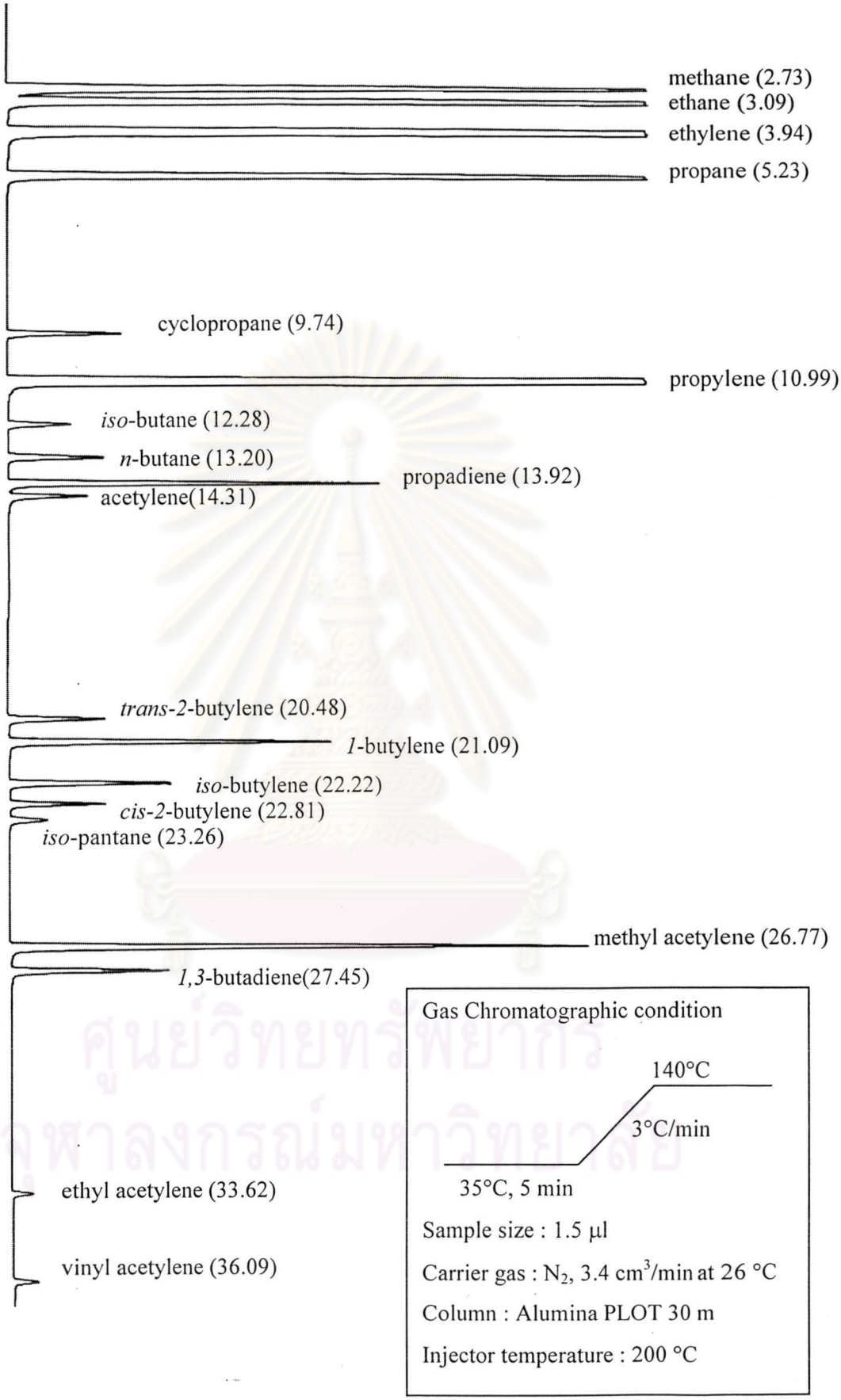

Figure A-1 Gas chromatogram of standard mixture C_4 gas.

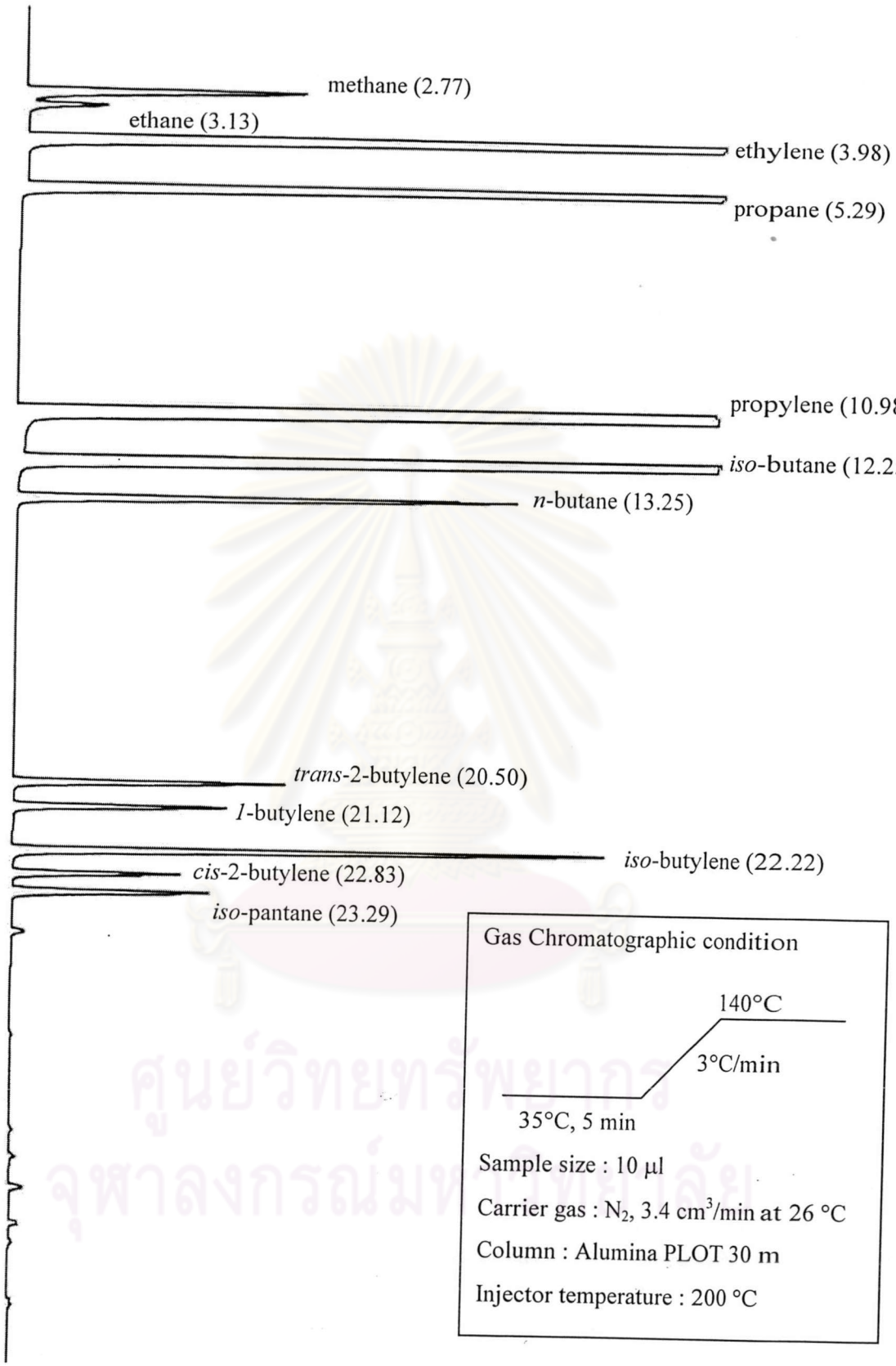

Figure A-2 Gas chromatogram of gas product from methanol conversion reaction on H-MOR (Si/Al ratio = 120) at 500°C (Condition: 0.4 g of catalyst, feed at GHSV of 2000 h^{-1}, T_{MeOH} = 29°C, time on stream 40 min.).

VITAE

Miss Jarurat Waitayawan was born on February 4, 1976 in Sakonnakhon. She received the B.Sc. Degree in Chemistry at Srinakharinwirot University in 1999. Since then, she has been a graduate student studying in the program of Petrochemistry and Polymer Science at Faculty of Science, Chulalongkorn University. During her graduate studies towards her M.Sc. degree, the Graduate School, Chulalongkorn University awarded her a research grant.