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APPENDIX A
SAMPLE OF CALCULATIONS

A-1 Calculation of Si/Al Atomic Ratio for Beta Zeolite Preparation

The calculation is based on weight of Sodium Aluminate (Al/NaOH = 0.78) in gel preparation.

Molecular Weight of Al = 26.9815

Molecular Weight of $NaAlO_2$ = 81097

Using Sodium Aluminate ($NaAlO_2$) 0.702 g as gel preparation.

$$\text{Mole of Al used} = \text{wt.} \times \frac{(\%)}{100} \times \frac{(\text{M.W. of Al})}{(\text{M.W. of } NaAlO_2)} \times \frac{(1\text{ mole})}{(\text{M.W. of Al})} \quad (A1.1)$$

$$= (0.702)(0.78)(1/81.97)$$

$$= 6.680\times10^{-3} \text{ mole}$$

For example, to prepare Beta zeolite at Si/Al atomic ratio of 80 by using Cataloid (SiO_2 30% wt in water) for silicon source.

Molecular Weight of Si = 28.0855

Molecular Weight of SiO_2 = 60.0843

Si/Al atomic ratio of 80

mole of SiO_2 required = $(6.680\times10^{-3})(80)$

= 0.5344 mole

amount of SiO_2 = (0.5344)(60.0843)

= 32.1090 g

amount of Cataloid = (100/30)(32.1090)

= 107.0301 g

This is the amount of $NaAlO_2$ and SiO_2 used in gel preparation.

A-2 Calculation of Platinum ion exchange

Platinum ion-exchange

Determine the amount of Pt into catalyst = 0.1 wt.%

The catalyst use = X g

So that : from the equation

Pt/(X+Pt)	=	0.1/100
100Pt	=	0.1(X+Pt)
(100-0.1)Pt	=	0.1X
thus Pt	=	(0.1X)/(100-0.1) g

use $Pt(NH_3)_4Cl_2.H_2O$ (Molecular Weight = 252.13, 55% Pt)

Weight of $Pt(NH_3)_4Cl_2.H_2O$ = [0.1X/(100-0.1)]×[100/55] g

A-3 NH_3 Temperature programmed Desorption Calculation

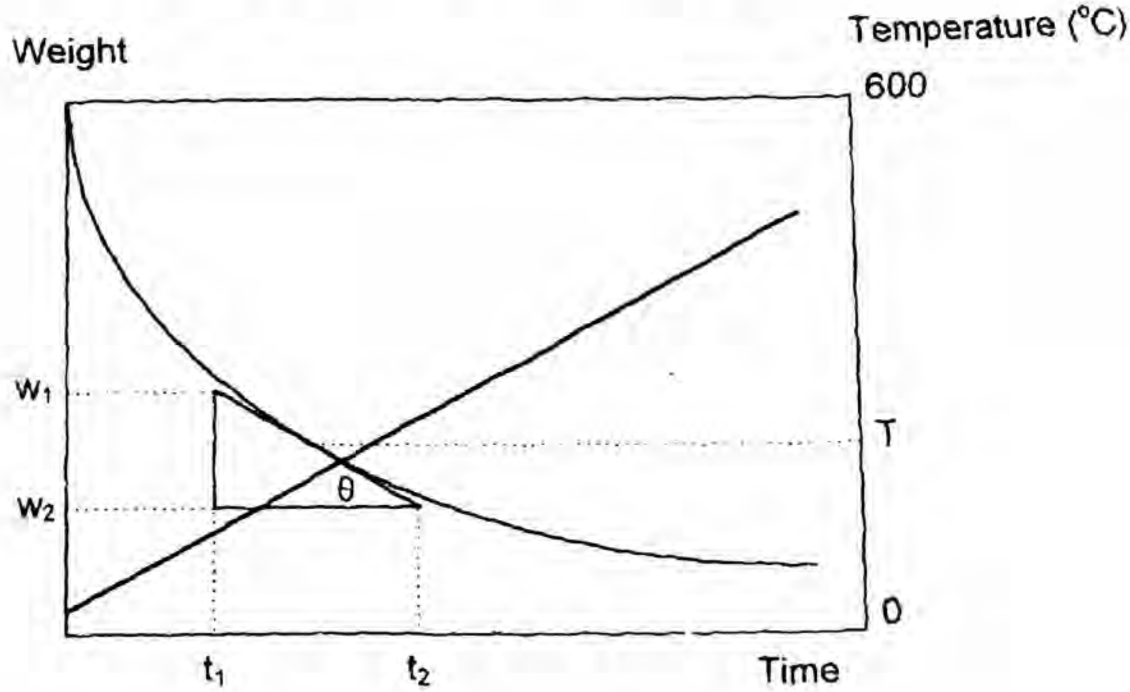


Figure A-1 Plot of weight loss and temperature versus time.

Chart speed	=	0.25 cm/min
Range	=	10 mg
W	=	weight of catalyst
W_W	=	weight of water
W_d	=	weight of dry catalyst = $W-W_W$

$$dw = 10 \text{ mg} \times (a/25 \text{ cm}) \qquad (A\text{-}2.1)$$

$$dt = 60 \text{ sec} \times (b/0.25 \text{ cm}) \qquad (A\text{-}2.2)$$

$$\frac{(dw/dt)}{W_d} = \frac{(10 \text{ mg} \times 0.25 \text{ cm} \times a)/(60 \text{ sec} \times 25 \text{ cm} \times b)}{W_d} \qquad (A\text{-}2.3)$$

Plot $\frac{(dw/dt)}{W_d}$ versus temperature

A-4 Calculation of Reactant Flow Rate

The catalyst used = 0.3000 g

packed catalyst into quartz reactor (inside diameter = 0.6 cm)

determine the average high of catalyst bed = H cm. So that,

Volume of bed= $\pi(0.3)^2 \times h$ cc-cat.

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

$$GHSV = \frac{\text{Volumetric flow rate}^1}{\text{Volume of bed}}$$

$$\begin{aligned}\text{Volumetric flow rate}^1 &= 2000 \times \text{Volume of bed} \\ &= 2000\pi(0.3)^2 \times H \quad \text{cc/h} \\ &= (2000\pi(0.3)^2 \times H)/60 \quad \text{cc/min}\end{aligned}$$

at STP condition :

$$\text{Volumetric flow rate} = \text{Volumetric flow rate}^1 \times (273.15+T)/273.15$$

Where T = room temperature, °C.

A-5 Calculation of conversion and selectivity of n-hexane isomerization

The n-hexane isomerization activity and selectivity was evaluated as follow :

$$\text{n-Hexane Conversion (\%)} = \frac{(\text{n-Hexane in} - \text{n-Hexane out})}{\text{n-Hexane in}} \times 100$$

$$\text{Selectivity (\%)} = \frac{\text{desired product}}{\text{all product}} \times 100$$

$$= \frac{\text{desired product} \times 100}{\text{n-hexane in} - \text{n-hexane out}}$$

For example : Pt/H-Beta (Si/Al = 50, 0.6 wt.% of Pt) by wet impregnate.

Reaction condition : Reaction temperature 250°C. GHSV = 1600 h^{-1}, 20 min time on stream.

From Figure A-5.1 : chromatogram from column Chemipack C_{18}

Chemipack C18 (feed)

Area of feed n-hexane = 36068580

From Figure A-6.1 : calibration curve of n-hexane

Mole of feed n-hexane = 6.12×10^{-6} mole

From Figure A-5.2 : Chromatogram from column Chemipack C18

Chemipack C18 (product at 20 min time on stream)

Area of 2,2-Dimethylbutane (2,2-DMB)	= 776311
Area of 2,3-Dimethylbutane (2,3-DMB)	= 13079795
Area of 2-Methylpentane (2-MP)	+
Area of 3-Methylpentane (3-MP)	= 6043714
Area of Hexane	= 13672563

From Figure A-6.2 - A-6.10 : calibration curve

Mole of 2,2-DMB	$= 1.5\times10^{-7}$	mole
Mole of 2,3-DMB	$= 2.3\times10^{-6}$	mole
Mole of 2-MP	+	
Mole of 3-MP	$= 9.5\times10^{-7}$	mole
Mole of Hexane	$= 2.6\times10^{-6}$	mole

So that :

n-Hexane conversion (%) $= \dfrac{(6.12\times10^{-6}-2.6\times10^{-6})}{6.12\times10^{-6}} \times 100$

$= 57.5$ %

Total mole of all product $= (6.12-2.6) \times10^{-6}$

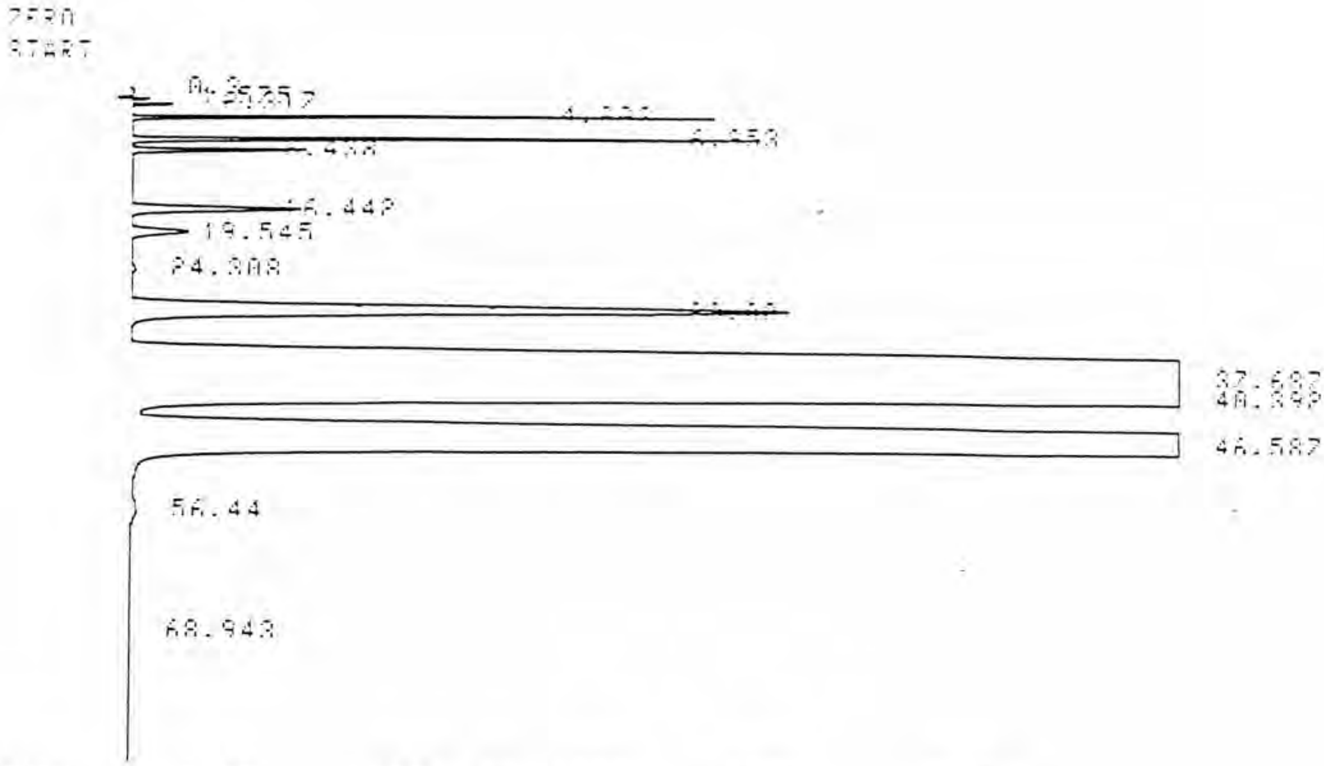
$= 3.52 \times10^{-6}$ mole

Total mole of desired product $= (150+2300+950) \times10^{-9}$

$= 3.4\times10^{-6}$ mole

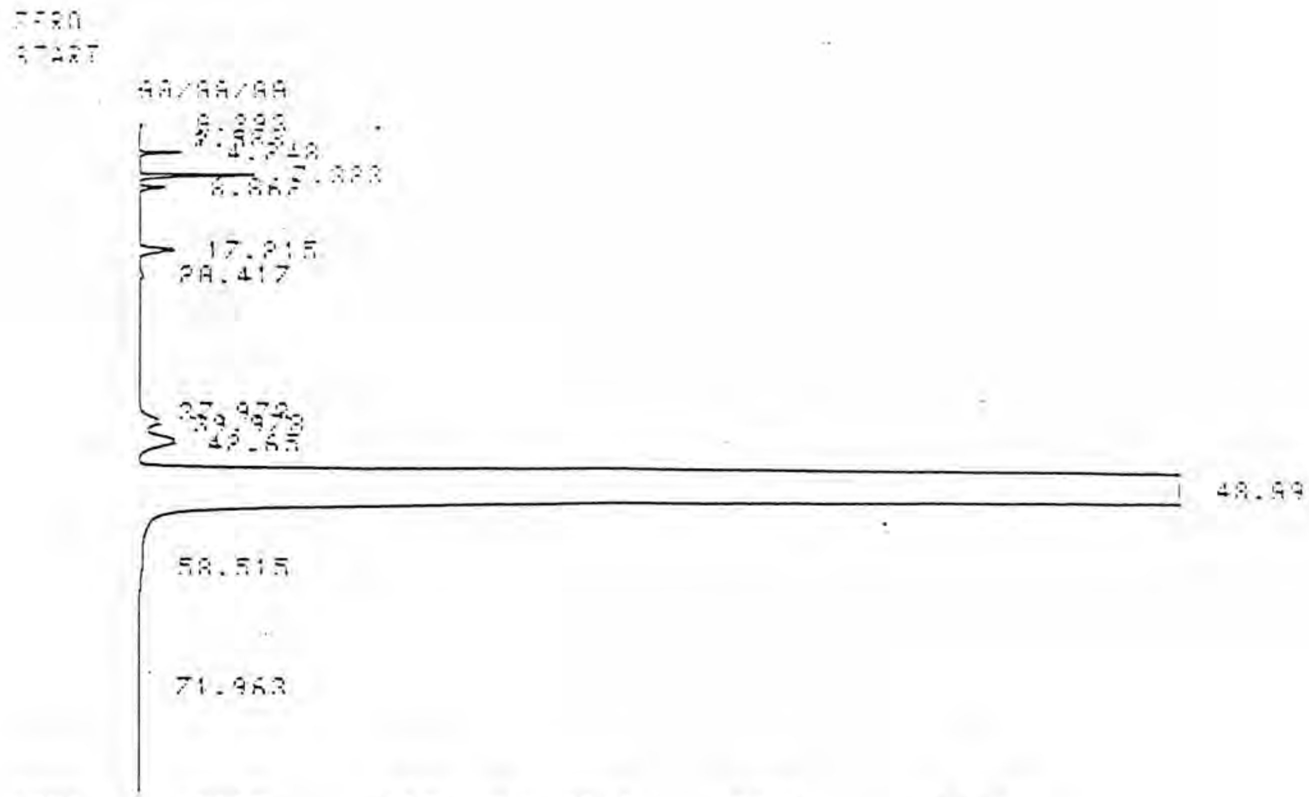
Selectivity (%) $= \dfrac{(3.4\times10^{-6})}{3.52\times10^{-6}} \times100$

$= 96.59$ %



PKNO	TIME	AREA	MK	IDNO	CONC	NAME
1	0.2	1407			0.0041	
2	1.575	4619			0.0135	
3	2.317	6912			0.0202	
4	4.003	119462			0.3498	
5	6.953	188856			0.553	
6	8.438	62188	V		0.1821	
7	16.442	113546			0.3325	
8	19.545	47623	V		0.1394	
9	24.308	6610			0.0194	
10	29.82	776311			2.2731	
11	37.687	13079795	V		38.2982	
12	40.392	6043714	V		17.6962	
13	46.587	13672563	V		40.0338	
14	56.44	23540	V		0.0689	
15	68.943	5371			0.0157	
	TOTAL	34152512			100	

Figure A-5.1 Chromatogram of product from Chemipack C18



PKNO	TIME	AREA	MK	IDNO	CONC	NAME
1	0.293	1617			0.0045	
2	1.888	695			0.0019	
3	2.5	288	V		0.0008	
4	4.248	10761			0.0297	
5	7.323	39258			0.1083	
6	8.862	10081	V		0.0278	
7	17.215	23758			0.0655	
8	20.417	5852			0.0161	
9	37.978	4283			0.0118	
10	39.978	32085	V		0.0885	
11	42.65	59926	V		0.1652	
12	48.09	36068580	SV		99.4553	
13	58.515	2891	T		0.008	
14	71.963	6053			0.0167	
	TOTAL	36266104			100	

Figure A-5.2 Chromatogram of feed from Chemipack C18

A-6 Calculation of partial vapour pressure of n-hexane

Equation:

$$Ln(P_{vp}/P_c) = (1-x)^{-1}[(VP\ A)x+(VP\ B)x^{1.5}+(VP\ C)x^3+(VP\ D)x^6] \qquad (4.1)$$

Where; x = 1-T/Tc

P_{vp} = vapour pressure, in bars

Pc = critical pressure, in bars

Tc = critical temperature, in Kelvins

T = temperature, in Kelvins

For n-hexane: VP A = -7.46765

VP B = 1.44211

VP C = -3.28222

VP D = -2.50941

Tc = 507.5 K

Pc = 30.1 bar

Set the temperature of water bath at 283 K

Then, x = 1-(283/507.5) = 0.442

$$\ln(Pvp/30.1)=(1-0.442)^{-1}[(-7.46765)(0.442)+(1.44211)(0.422)^{1.5}$$
$$+(-3.28222)(0.442)^3+(-2.50941)(0.442)^6]$$
$$= -5.7025$$

∴ Pvp = 0.100 bar

partial vapour pressure of n- hexane at 10 °C = (0.10/1.013)×100

= 9.87 %

A-7 Calibration curve for GC with column Chemipack C18

Figure A-6.1 Calibration curve of n-Hexane

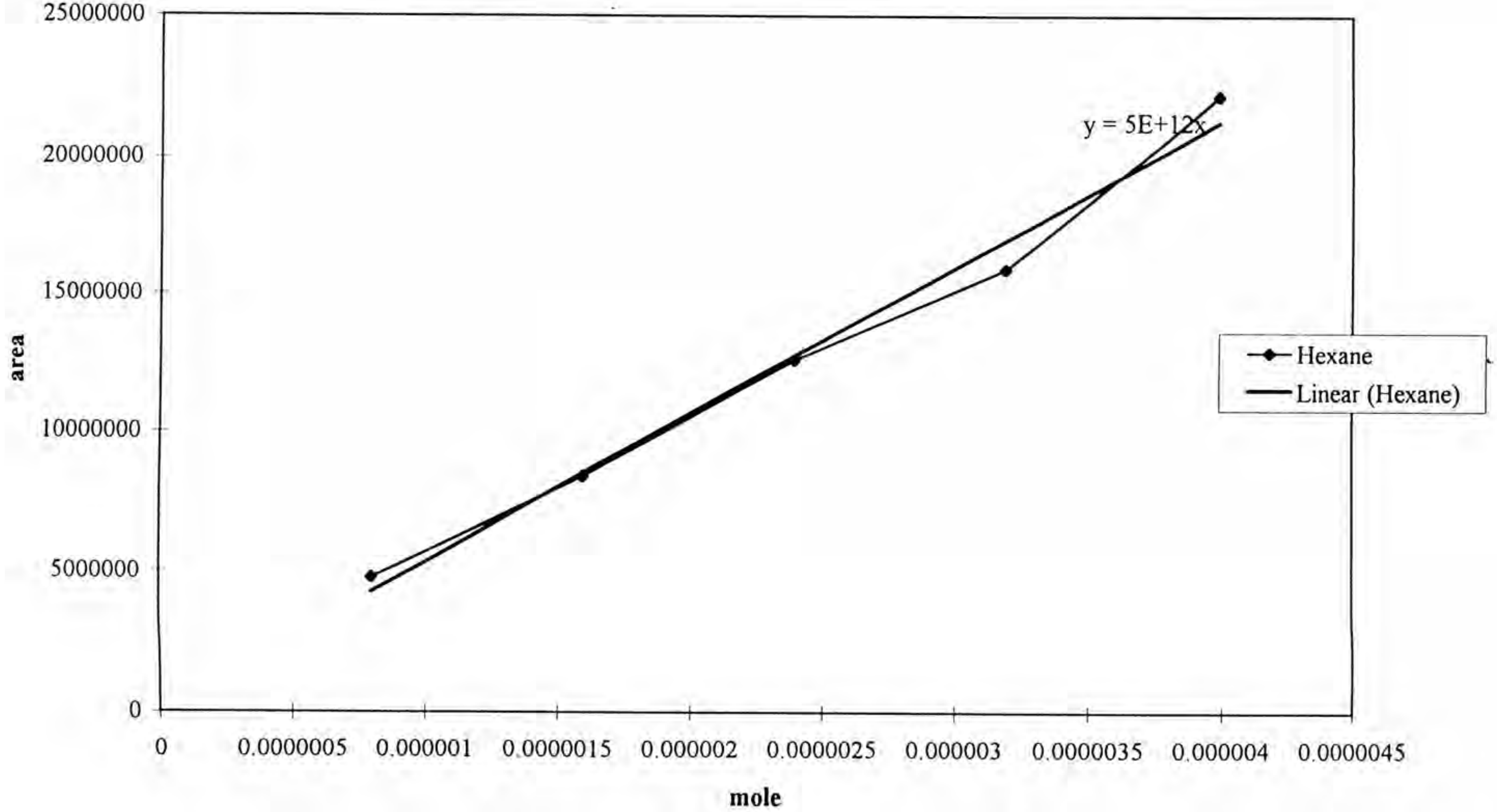


Figure A-6.2 Calibration curve of 2,2-dimethylbutane(2,2-DMB)

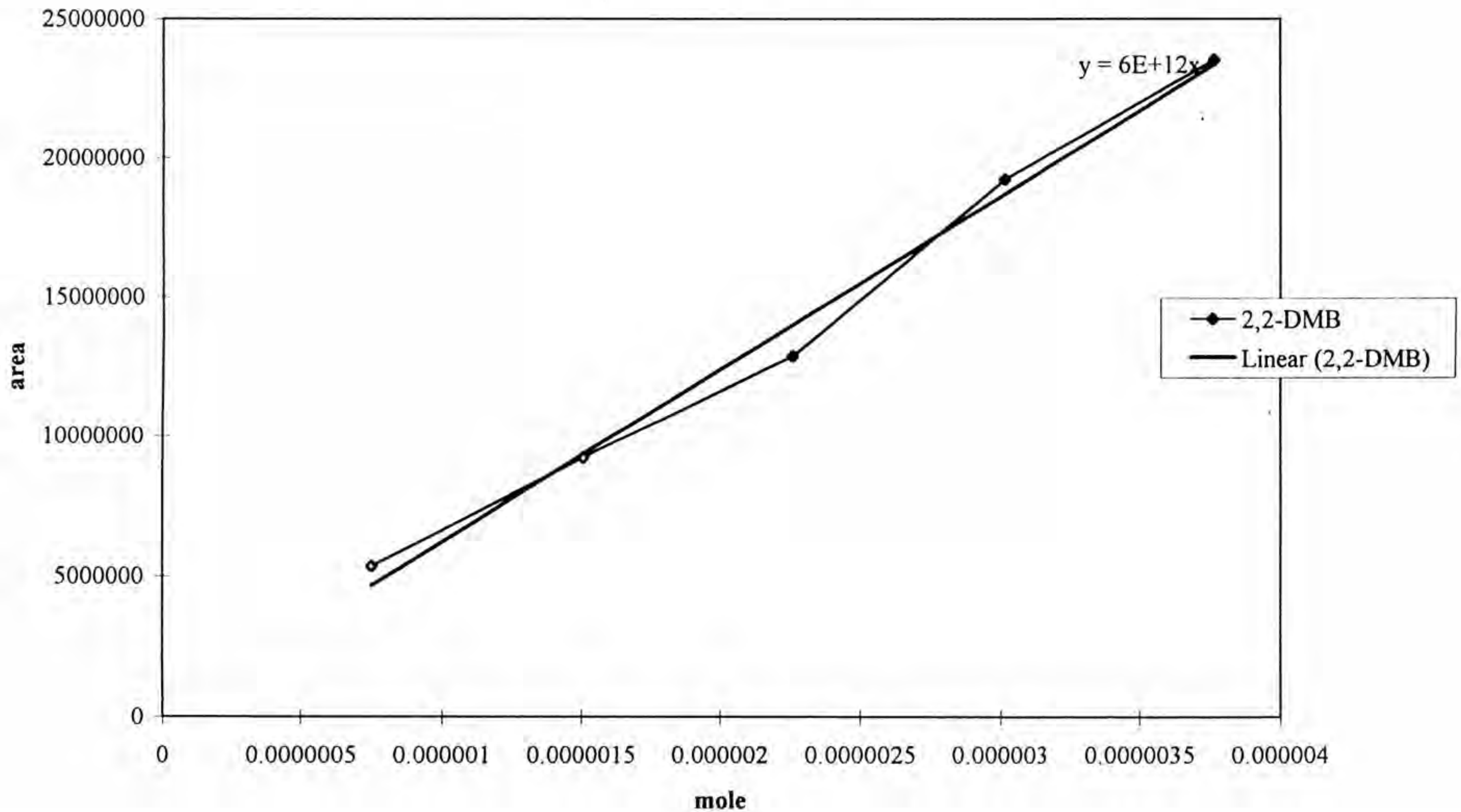


Figure A-6.3 Calibration curve of 2,3-dimethylbutane(2,3-DMB)

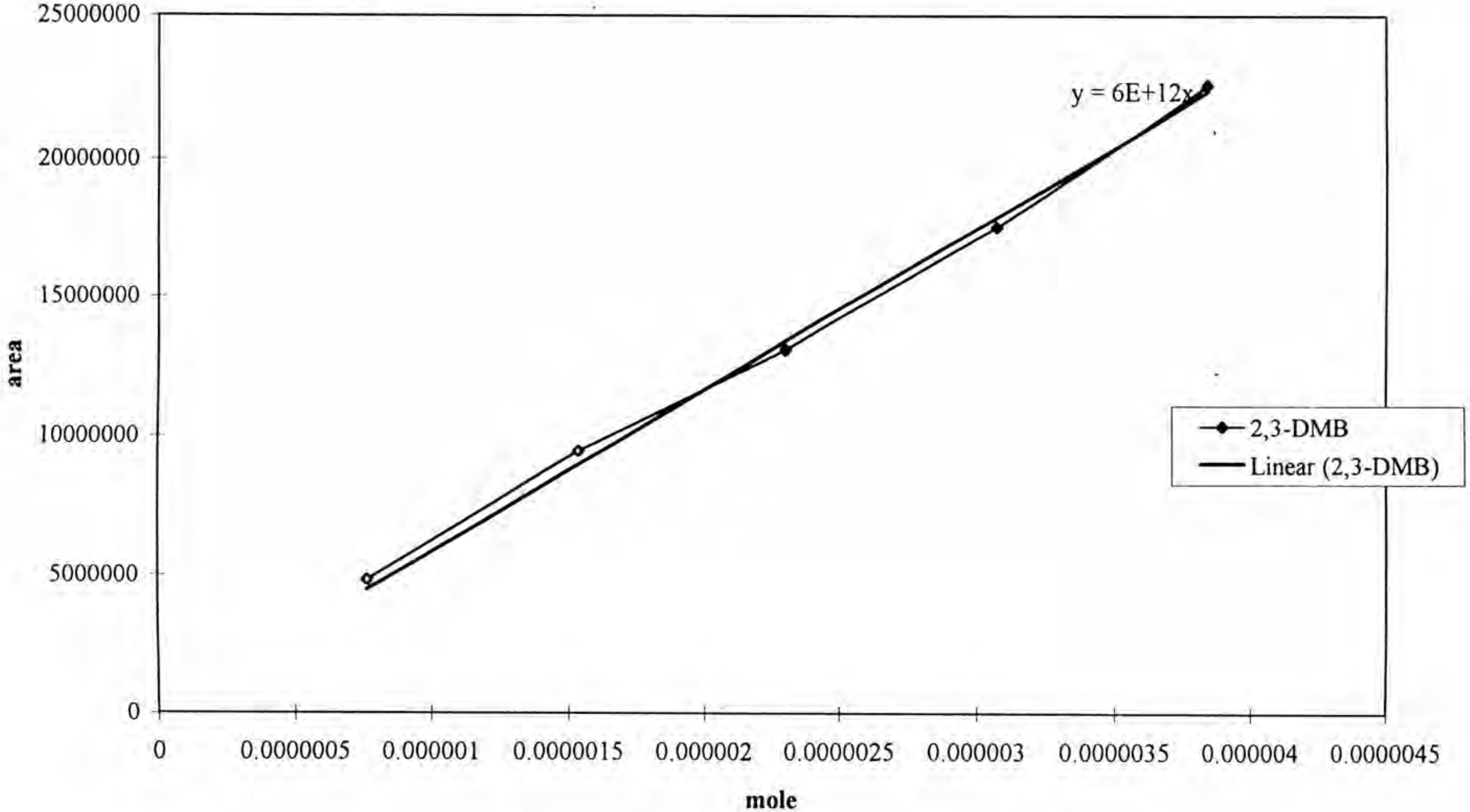


Figure A-6.4 Calibration curve of 2-methylpentane (2-MP)

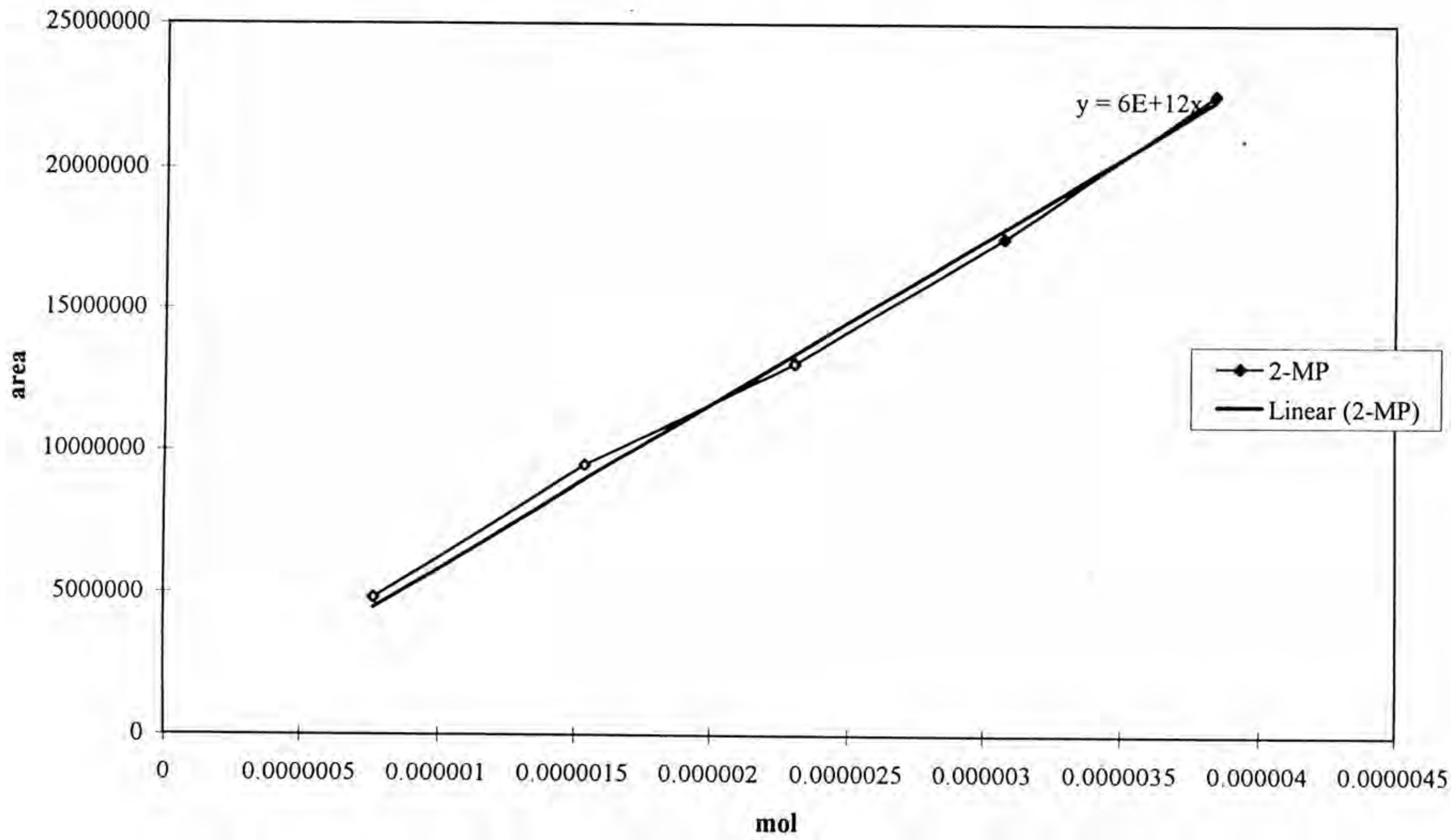


Figure A-6.5 Calibration curve of 3-methylpentane (3-MP)

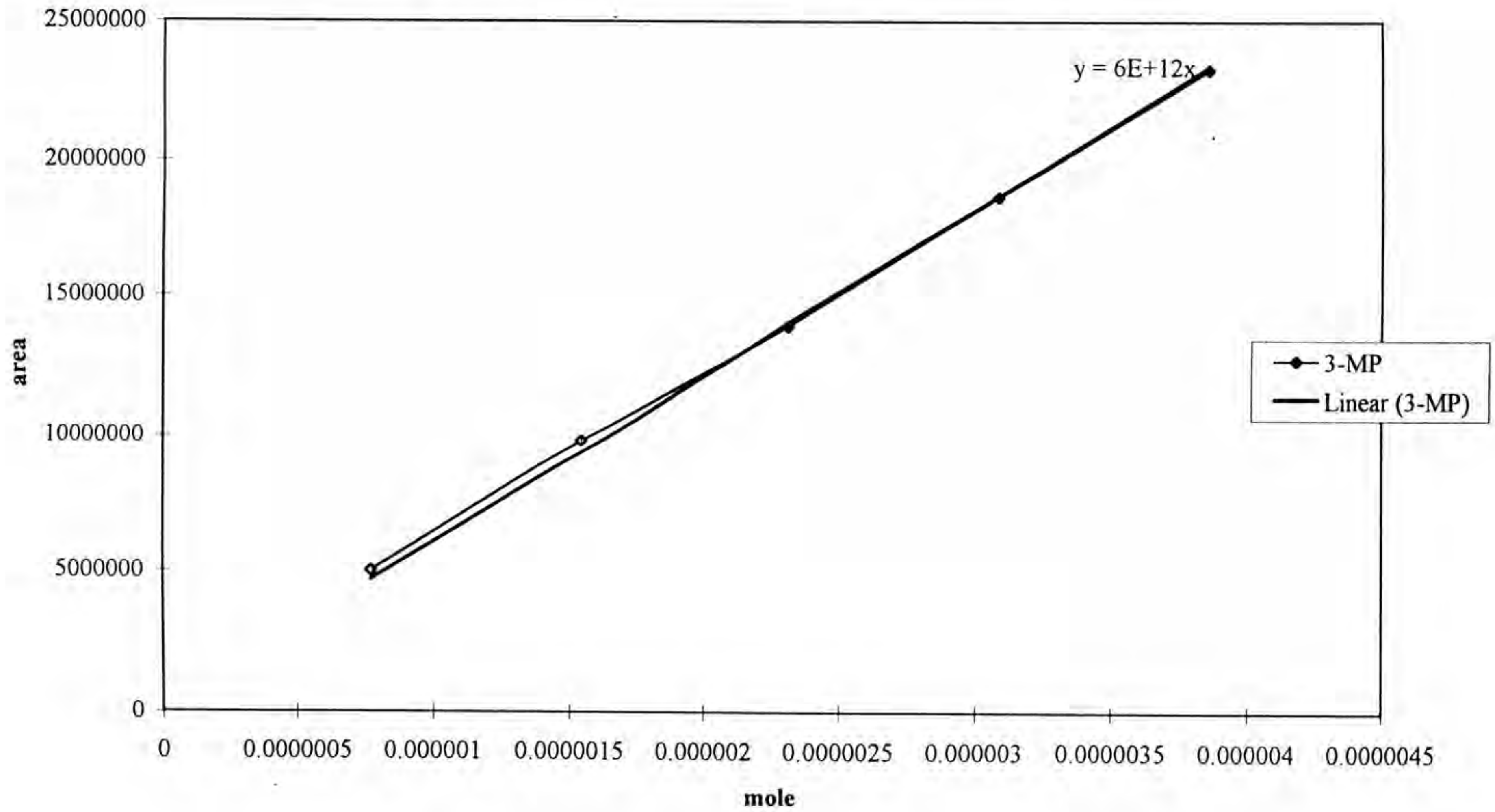


Figure A-6.6 Calibration curve of Ethylene

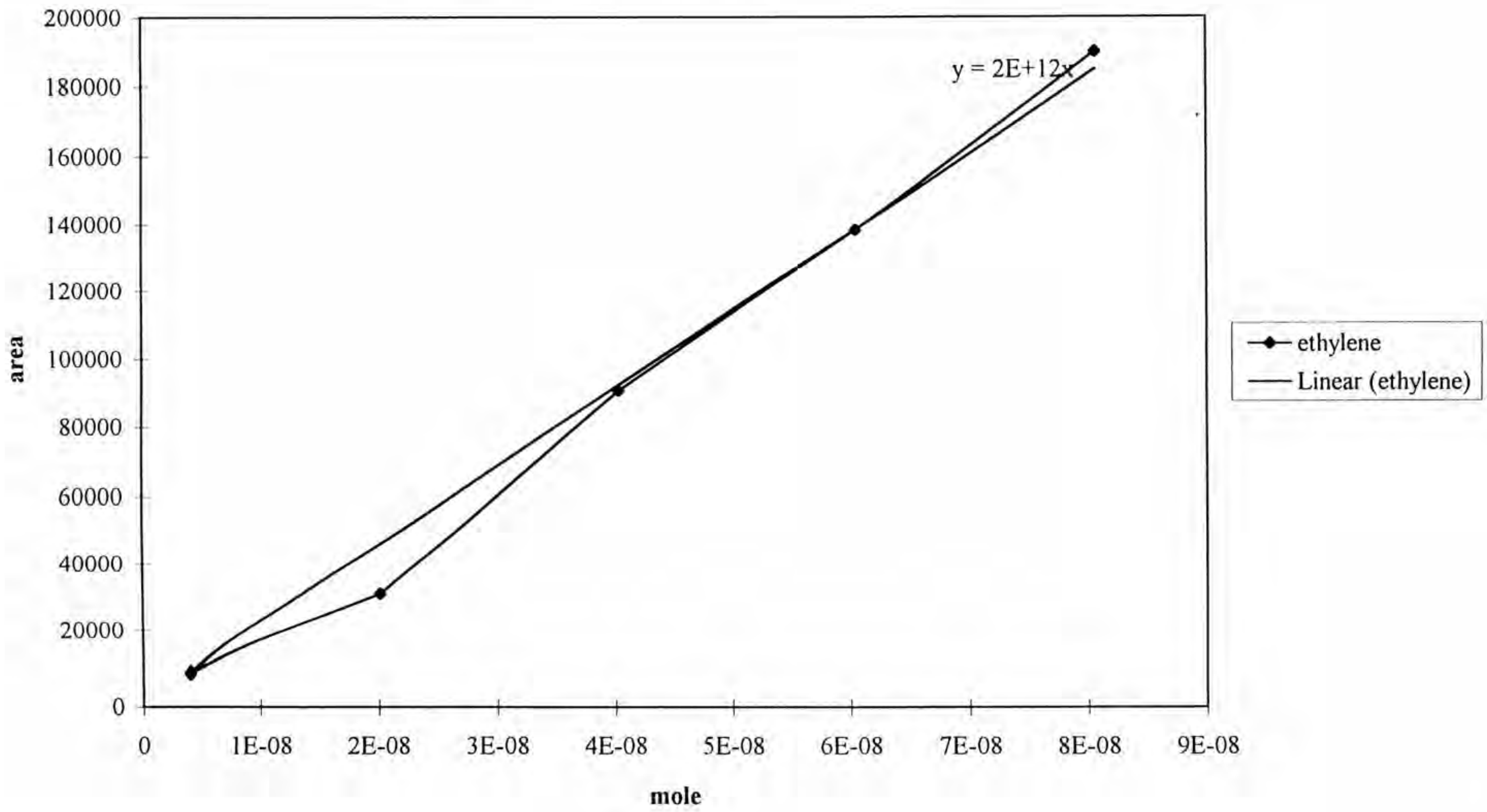


Figure A-6.7 Calibration curve of Propylene

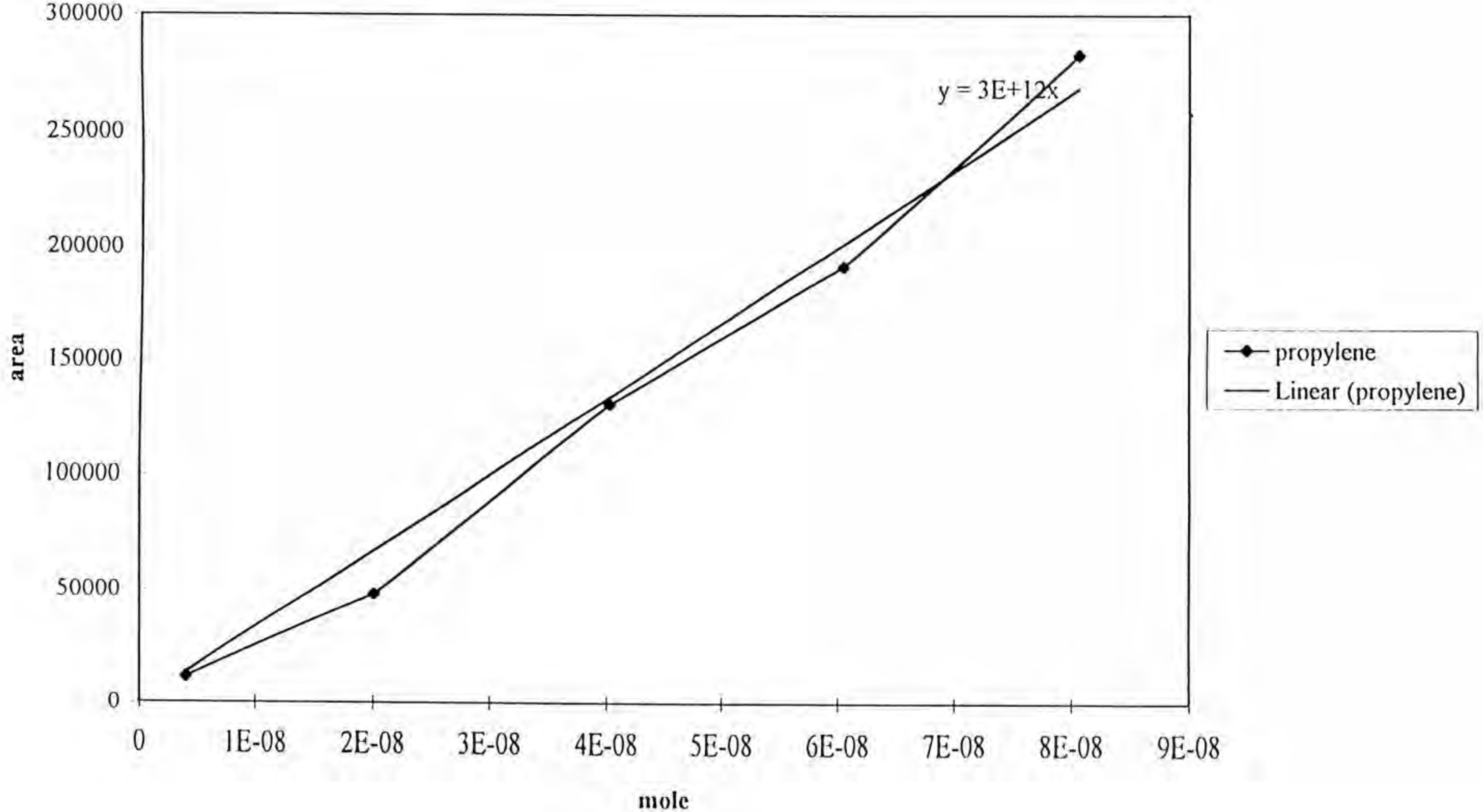


Figure A-6.8 Calibration curve of 1-Butene

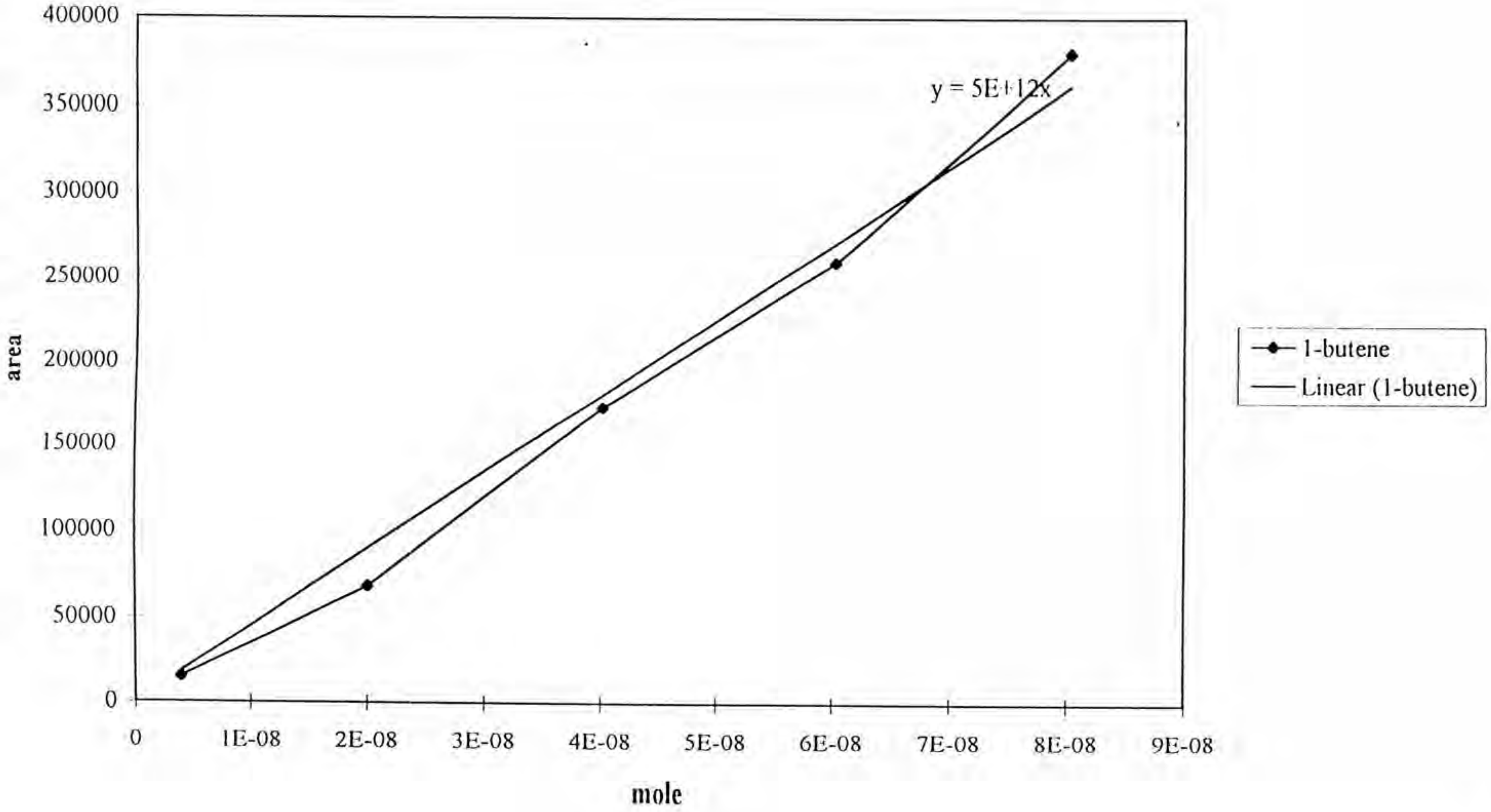
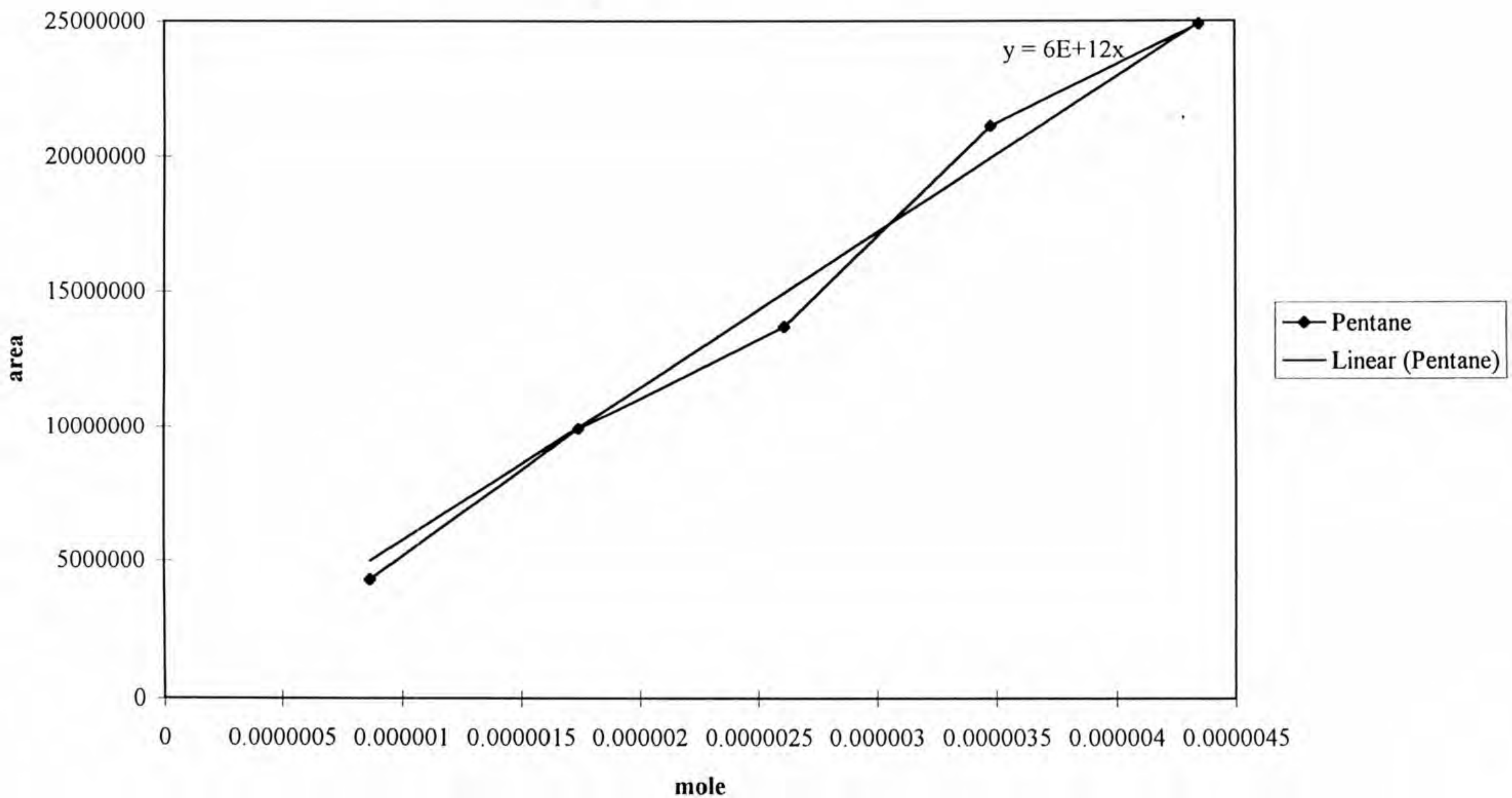


Figure A-6.9 Calibration curve of Pentane



VITA

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