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NOMENCLATURE

a_i activity of i-component

C_p heat of capacity (J/^oK mol)

C_L molar concentration of the free active sites referred to the unit mass of the catalyst (mol/mass of catalyst)

C_i molar concentration of i-component (mole/mass of catalyst)

G Gibbs free energy (cal/mol or J/mol)

G_R^o standard Gibbs free energy of reaction (kJ/mol)

G_e^o standard Gibbs free energy of combustion (kJ/mol)

G_f^o standard Gibbs free energy of formation (kJ/mol)

H heat of reaction (KJ/mol)

H_c^o standard heat of combustion (KJ/mol)

H_d^o standard heat of dissociation (KJ/mol)

H_f^o standard heat of formation (KJ/mol)

K equilibrium constant

k' adsorption rate constant

k'' desorption rate constant

k_s' rate constant for direct reactions in the adsorbed phase

k_s'' rate constant for reverse reactions in the adsorbed phase

P_i partial pressure of i-component (atm)

P total pressure (atm)

r rate of reaction

S^o standard entropy (J/^oK mol)

S number of active sites

T temperature

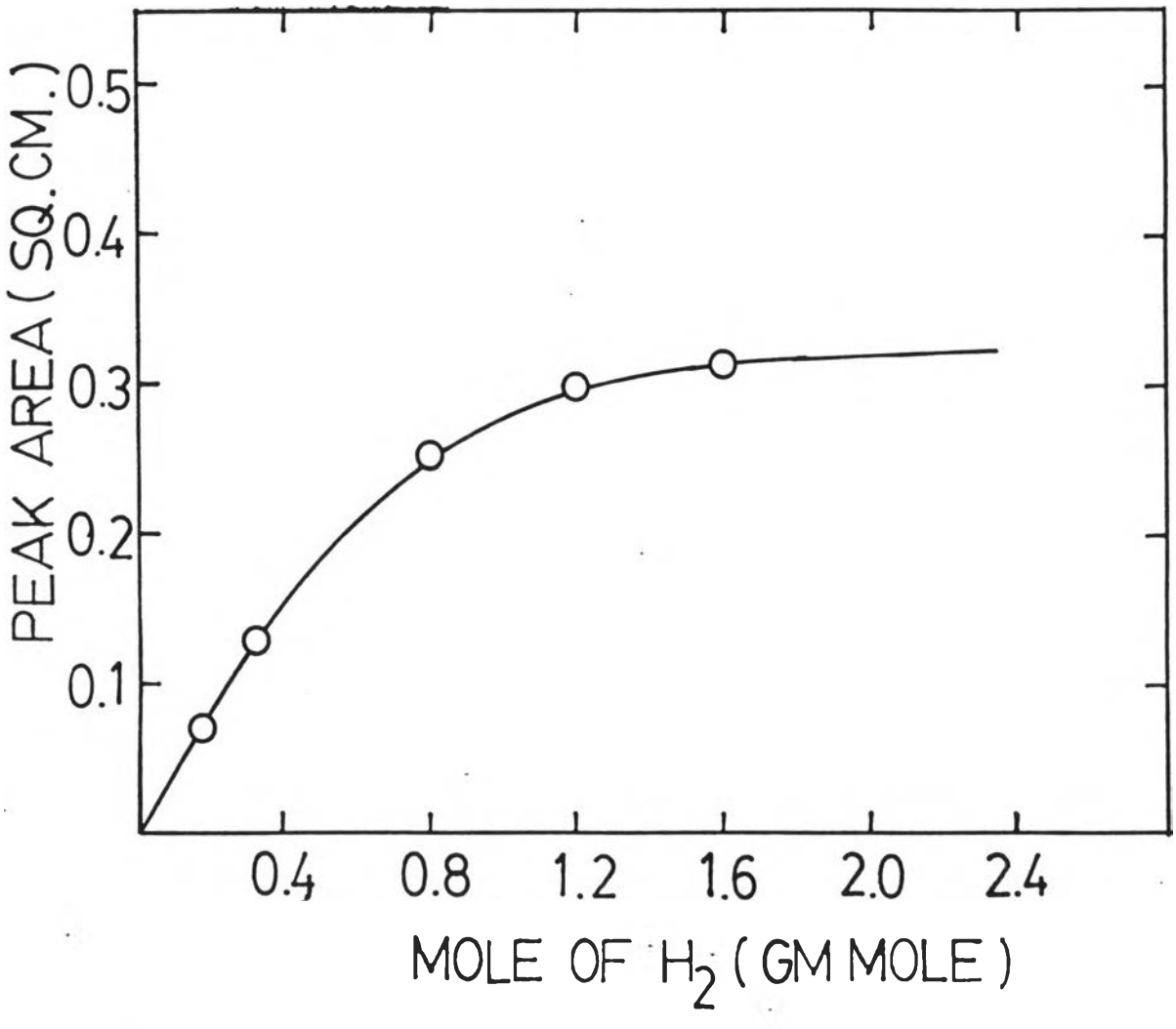
W weight of catalyst (gm)

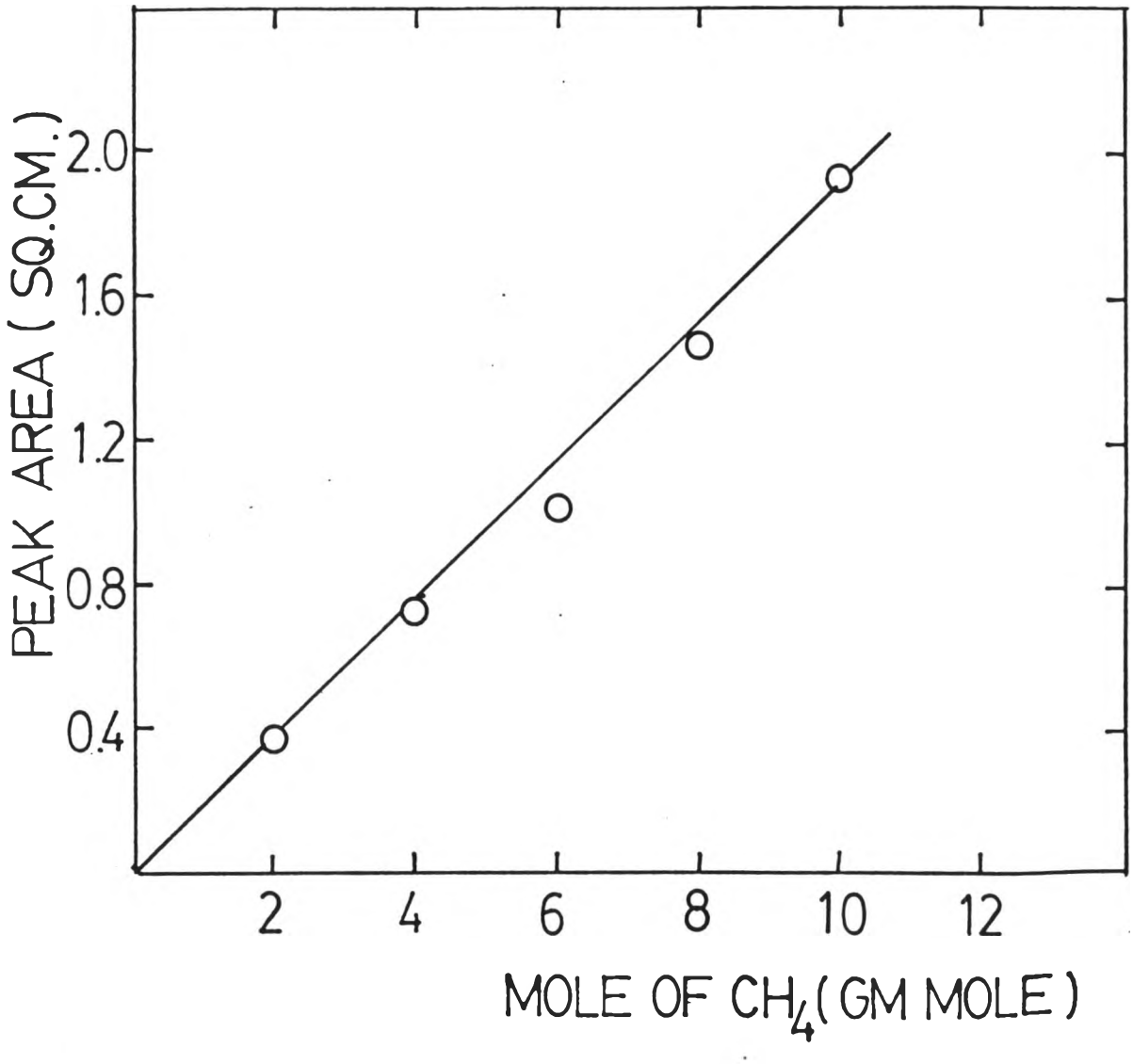
X	mole fraction at equilibrium
ρ	density (mass/volume)
γ_i	fugacity coefficient of i-component

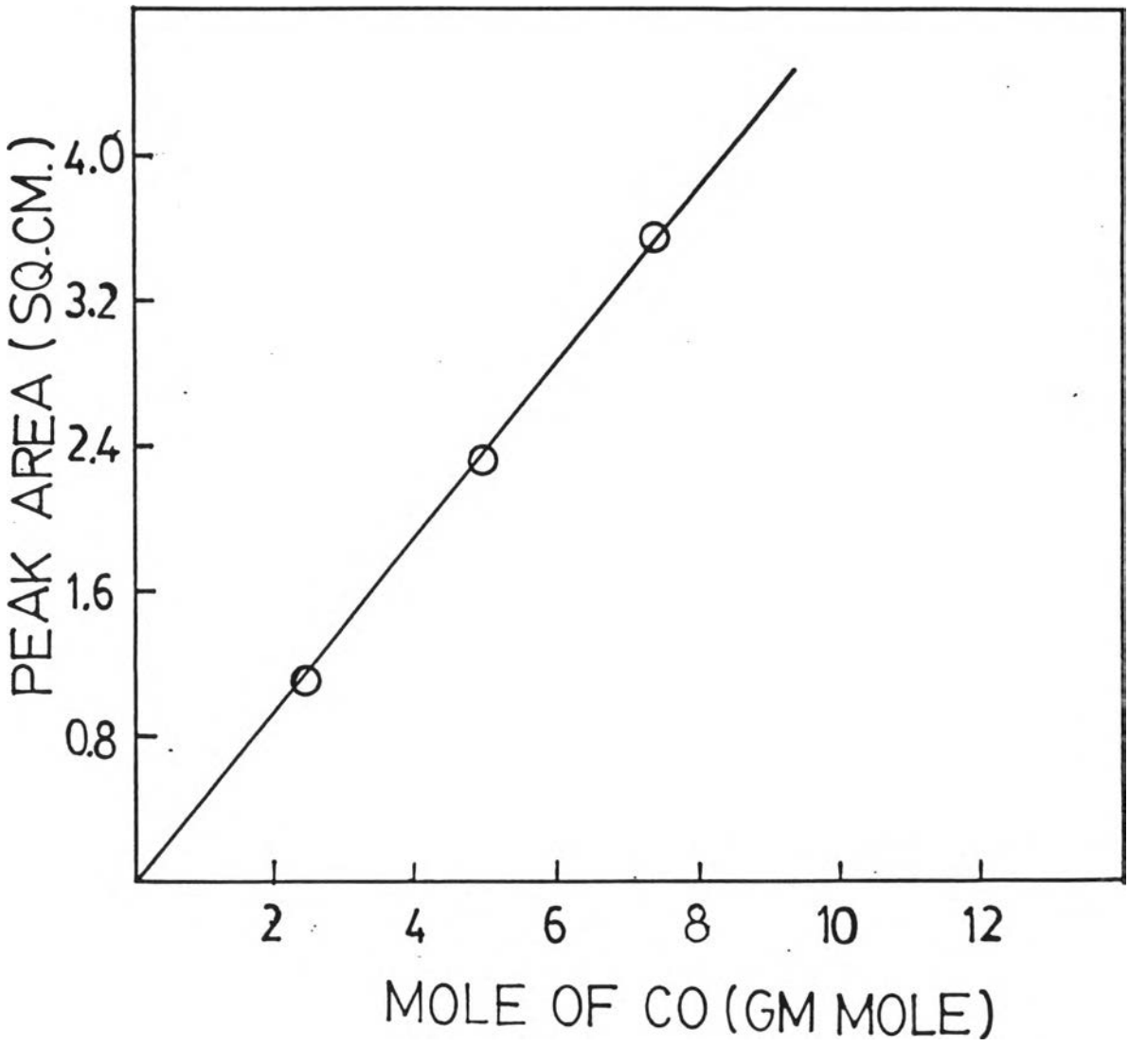
APPENDIX A

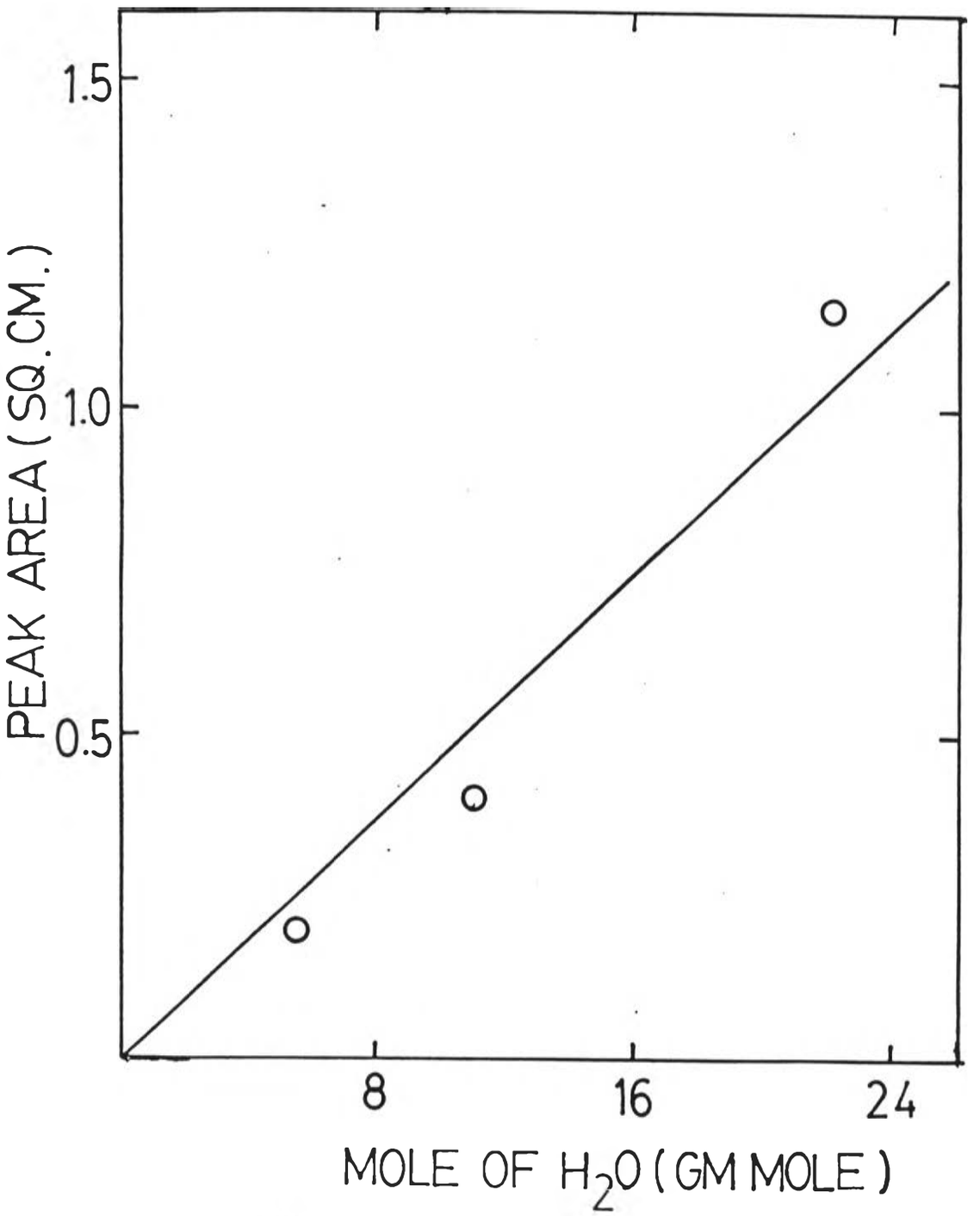
The following calibration curves obtained from Shimadzu Gas Chromatography model 8AIT (TCD) with the operations :

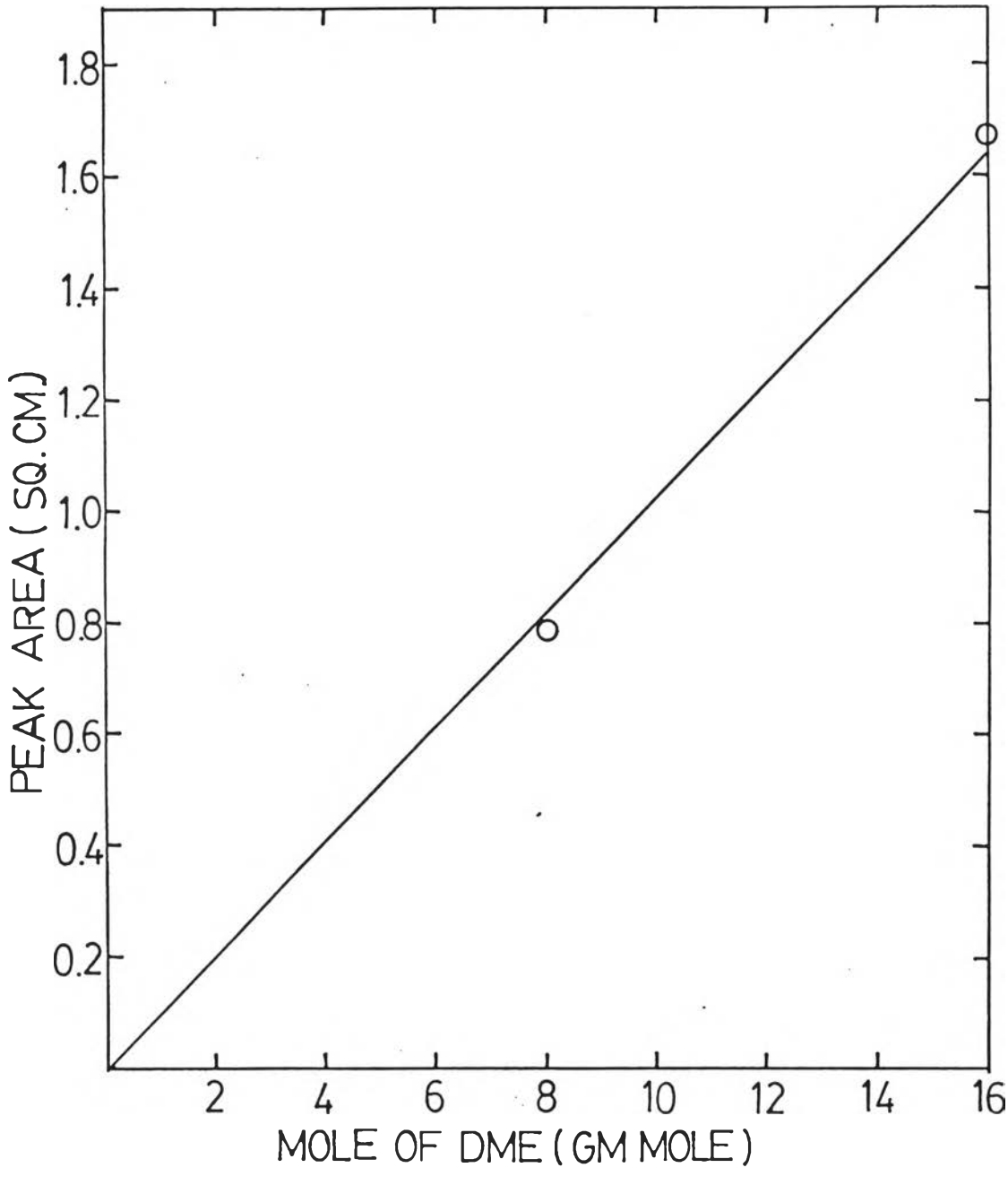
Inj/DET temperature	:	$150^{o}C$
Column temperature	:	$125^{o}C$
Carrier gas	:	He
Carrier gas pressure of MS-5A	:	3.4-3.5 atg
Carrier gas pressure of PT	:	5 atg
Flow rate of carrier gas in MS-5A column	:	32 ml/min
Flow rate of carrier gas in PT column	:	60 ml/min
MS-5A detected	:	CH_4 and CO
PT detected	:	CO_2, DME, C_2H_6, C_3H_8, H_2O and MeOH
Polarity MS-5A	:	+
Polarity PT	:	-

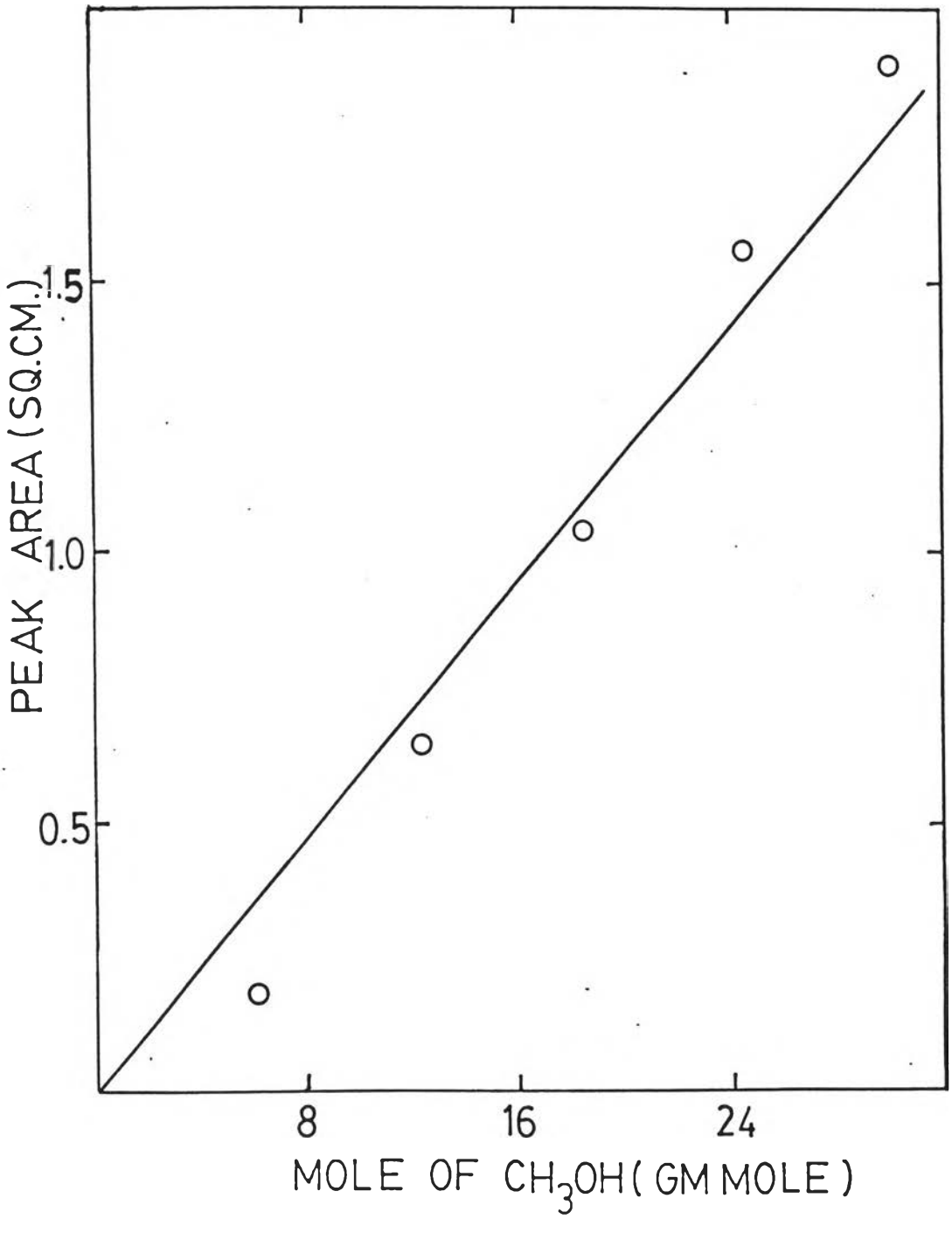

PEAK AREA (SQ. CM.)
0.5
0.4
0.3
0.2
0.1
0.4
0.8
1.2
1.6
2.0
2.4
MOLE OF H_2 (GM MOLE)

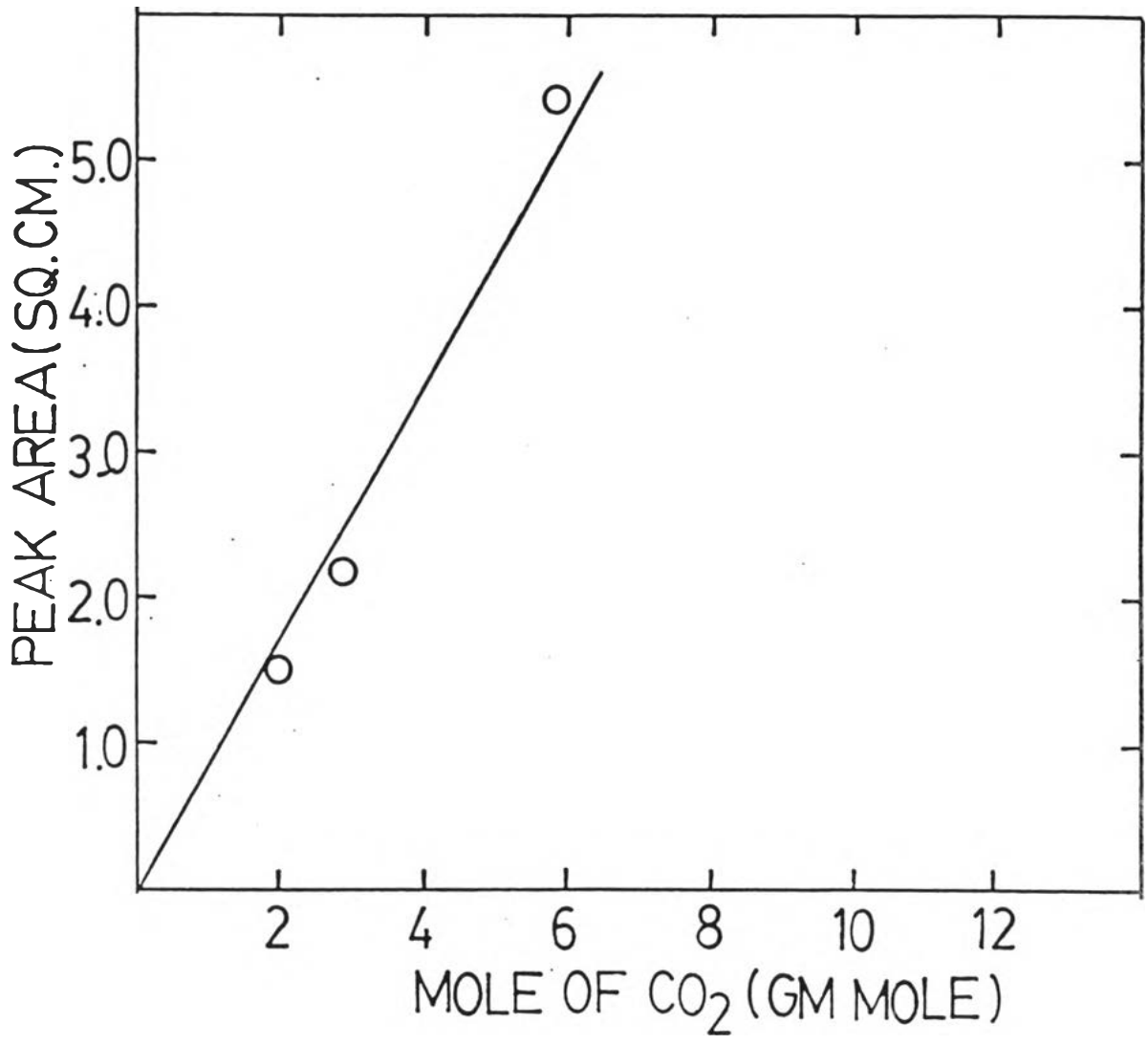

PEAK AREA (SQ.CM.)
2.0
1.6
1.2
0.8
0.4
2
4
6
8
10
12
MOLE OF CH_4 (GM MOLE)


PEAK AREA (SQ.CM.)
4.0
3.2
2.4
1.6
0.8
2
4
6
8
10
12
MOLE OF CO (GM MOLE)


1.5
1.0
0.5
PEAK AREA (SQ. CM.)
8
16
24
MOLE OF H_2O (GM MOLE)


PEAK AREA (SQ. CM.)
1.8
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
2
4
6
8
10
12
14
16
MOLE OF DME (GM MOLE)


PEAK AREA (SQ.CM.)
1.5
1.0
0.5
8
16
24
MOLE OF CH_3OH (GM MOLE)


PEAK AREA (SQ.CM.)
5.0
4.0
3.0
2.0
1.0
2
4
6
8
10
12
MOLE OF CO_2 (GM MOLE)

APPENDIX B

EXPERIMENTAL RESULTS OF CATALYST NO.1

Reaction Condition P = 40 atg

GHSV = 2000 hr^{-1}

Reaction Temperature (^{o}C)		208	237	265	296
Product Selectivity	CH_3OH (%)	52.64	75.68	65.60	46.01
	CO_2 (%)	14.47	9.46	14.22	21.57
	CH_4 (%)	-	-	2.13	6.38
	C_2H_6 (%)	-	-	1.37	4.28
	C_3H_8 (%)	-	-	1.31	2.97
	C_2H_4 (%)	-	-	-	-
	C_3H_6 (%)	-	-	-	-
	CH_3OCH_3 (%)	-	5.40	8.25	17.89
	other H.C(%)	32.89	9.46	7.12	0.90
	total H.C(%)	32.89	9.46	11.93	14.53
Conversion of CO (%)		4.057	7.89	20.87	33.75
Space-Time Yield of CH_3OH, (mol/l-cat.hr)		0.6356	1.7771	4.0746	4.6215
Space-Time Yield of DME (mol/l-cat.hr)		-	0.0634	0.2562	0.8985

Reaction Condition P = 40 atg

GHSV = 4000 hr^{-1}

Reaction Temperature (°C)		207	236	263	293
Product Selectivity	CH_3OH (%)	52.63	68.57	56.98	52.29
	CO_2 (%)	13.16	10.0	12.29	18.95
	CH_4 (%)	-	-	2.68	1.04
	C_2H_6 (%)	-	-	1.23	1.96
	C_3H_8 (%)	-	-	-	1.27
	C_2H_4 (%)	-	-	-	-
	C_3H_6 (%)	-	-	-	-
	CH_3OCH_3 (%)	-	-	5.59	14.38
	other H.C(%)	34.21	21.43	21.23	10.11
	total H.C(%)	34.21	21.43	25.14	14.38
Conversion of CO (%)		2.12	3.59	9.023	15.15
Space-Time Yield of CH_3OH, (mol/l-cat.hr)		0.6641	1.4653	3.0603	4.7154
Space-Time Yield of DME (mol/l-cat.hr)		-	-	0.1501	0.6484

Reaction Condition P = 40 atg

GHSV = 8000 hr^{-1}

Reaction Temperature (^{o}C)		204	235	267	295
Product Selectivity	CH_3OH (%)	33.34	56.53	46.23	46.29
	CO_2 (%)	9.52	13.04	10.38	21.07
	CH_4 (%)	-	-	1.5	4.21
	C_2H_6 (%)	-	-	0.66	1.78
	C_3H_8 (%)	-	-	-	2.31
	C_2H_4 (%)	-	-	-	-
	C_3H_6 (%)	-	-	-	-
	CH_3OCH_3 (%)	-	-	5.66	11.28
	other H.C(%)	57.14	30.43	35.58	13.06
	total H.C(%)	57.14	30.43	37.74	21.36
Conversion of CO (%)		2.3	2.75	11.3	18.53
Space-Time Yield of CH_3OH, (mol/l-cat.hr)		0.9129	1.8507	6.219	10.2114
Space-Time Yield of DME (mol/l-cat.hr)		-	-	0.3807	1.2442

Reaction Condition P = 40 atg

GHSV = 16,000 hr^{-1}

Reaction Temperature (^{o}C)		203	232	266	295
Product Selectivity	CH_3OH (%)	12.5	40.23	54.24	47.86
	CO_2 (%)	18.75	9.77	13.56	15.38
	CH_4 (%)	-	-	-	4.68
	C_2H_6 (%)	-	-	-	1.30
	C_3H_8 (%)	-	-	-	-
	C_2H_4 (%)	-	-	-	-
	C_3H_6 (%)	-	-	-	-
	CH_3OCH_3 (%)	-	-	10.17	8.55
	other H.C(%)	68.75	50.00	22.03	22.23
	total H.C(%)	68.75	50.00	22.03	28.21
Conversion of CO (%)		0.88	1.94	3.29	7.17
Space-Time Yield of CH_3OH, (mol/l-cat.hr)		0.2619	1.8582	4.2488	8.1704
Space-Time of Yield of DME (mol/l-cat.hr)		-	-	0.3983	0.7298

Reaction Condition P = 30 atg

GHSV = 2000 hr^{-1}

Reaction Temperature (°C)		204	234	263	294
Product Selectivity	CH_3OH (%)	7.87	31.28	44.19	36.02
	CO_2 (%)	1.12	5.35	9.88	22.46
	CH_4 (%)	-	-	2.25	2.99
	C_2H_6 (%)	-	-	0.81	2.03
	C_3H_8 (%)	-	-	-	1.65
	C_2H_4 (%)	-	-	-	-
	C_3H_6 (%)	-	-	-	-
	CH_3OCH_3 (%)	-	4.11	8.14	17.8
	other H.C(%)	91.01	59.26	34.73	17.05
	total H.C(%)	91.01	59.26	37.79	23.72
Conversion of CO (%)		19.16	14.34	18.81	23.71
Space-Time Yield of CH_3OH, (mol/l-cat.hr)		0.44	1.3350	2.4739	2.5418
Space-Time of Yield of DME (mol/l-cat/hr)		-	0.0877	0.2278	0.6280

Reaction Condition P = 30 atg

GHSV = 4000 hr^{-1}

Reaction Temperature (^{o}C)		205	236	267	295
Product Selectivity	CH_3OH (%)	61.54	68.75	56.98	44.68
	CO_2 (%)	19.23	15.625	18.6	26.6
	CH_4 (%)	-	-	5.58	6.75
	C_2H_6 (%)	-	-	1.63	2.34
	C_3H_8 (%)	-	-	-	1.28
	C_2H_4 (%)	-	-	-	-
	C_3H_6 (%)	-	-	-	-
	CH_3OCH_3 (%)	-	-	6.98	1.42
	other H.C(%)	19.23	15.625	10.23	16.93
	total H.C(%)	19.23	15.625	17.44	27.3
Conversion of CO (%)		1.63	3.66	10.32	16.18
Space-Time Yield of CH_3OH, (mol/l-cat.hr)		0.5971	1.4978	3.5002	4.3031
Space-Time of Yield of DME (mol/l-cat.hr)		-	-	0.2144	0.0684

Reaction Condition P = 30 atg

GHSV = 8000 hr^{-1}

Reaction Temperature (°C)		202	238	267	294
Product Selectivity	CH_3OH (%)	14.28	60.87	58.54	49.03
	CO_2 (%)	5.36	10.87	13.41	19.35
	CH_4 (%)	-	-	-	5.17
	C_2H_6 (%)	-	-	-	1.82
	C_3H_8 (%)	-	-	-	-
	C_2H_4 (%)	-	-	-	-
	C_3H_6 (%)	-	-	-	-
	CH_3OCH_3 (%)	-	-	9.76	14.19
	other H.C(%)	80.36	28.26	18.29	10.44
	total H.C(%)	80.36	28.26	18.29	17.43
Conversion of CO (%)		3.52	3.51	5.46	9.996
Space-Time Yield of CH_3OH, (mol/l-cat.hr)		0.5984	2.5435	3.8051	5.8346
Space-Time of Yield of DME (mol/l-cat.hr)		-	-	0.3172	0.8443

Reaction Condition P = 30 atg

GHSV = 16000 hr^{-1}

Reaction Temperature (°C)		202	236	266	296
Product Selectivity	CH_3OH (%)	13.33	26.92	48.0	45.33
	CO_2 (%)	10.0	7.70	12.0	18.67
	CH_4 (%)	-	-	-	6.48
	C_2H_6 (%)	-	-	-	-
	C_3H_8 (%)	-	-	-	-
	C_2H_4 (%)	-	-	-	-
	C_3H_6 (%)	-	-	-	-
	CH_3OCH_3 (%)	-	-	-	13.33
	other H.C(%)	76.67	65.38	40.0	16.19
	total H.C(%)	76.67	65.38	40.0	22.67
Conversion of CO (%)		1.79	3.23	3.0189	4.84
Space-Time Yield of CH_3OH, (mol/l-cat.hr)		0.5681	2.0703	3.4502	5.2237
Space-Time Yield of DME (mol/l-cat.hr)		-	-	-	0.7681

Reaction Condition P = 20 atg

GHSV = 2000 hr^{-1}

Reaction Temperature (°C)		208	234	268	295
Product Selectivity	CH_3OH (%)	36.36	53.33	46.86	26.63
	CO_2 (%)	9.09	11.11	19.92	28.26
	CH_4 (%)	-	-	4.26	3.89
	C_2H_6 (%)	-	-	1.70	3.04
	C_3H_8 (%)	-	-	-	2.04
	C_2H_4 (%)	-	-	-	-
	C_3H_6 (%)	-	-	-	-
	CH_3OCH_3 (%)	-	4.45	11.71	17.39
	other H.C(%)	54.55	31.11	15.55	18.75
	total H.C(%)	54.55	31.11	21.51	27.72
Conversion of CO (%)		2.75	5.29	10.77	20.08
Space-Time Yield of CH_3OH, (mol/l-cat.hr)		0.2976	0.8396	1.5020	1.5915
Space-Time Yield of DME (mol/l-cat/hr)		-	0.035	0.1877	0.5196

Reaction Condition P = 20 atg

GHSV = 4000 hr^{-1}

Reaction Temperature (°C)		206	234	265	294
Product Selectivity	CH_3OH (%)	33.33	58.33	46.16	26.97
	CO_2 (%)	10.0	12.5	16.35	25.84
	CH_4 (%)	-	-	4.64	11.67
	C_2H_6 (%)	-	-	-	1.57
	C_3H_8 (%)	-	-	-	-
	C_2H_4 (%)	-	-	-	-
	C_3H_6 (%)	-	-	-	-
	CH_3OCH_3 (%)	-	-	7.69	15.73
	other H.C(%)	56.67	29.17	25.16	18.22
	total H.C(%)	56.67	29.17	29.8	31.46
Conversion of CO (%)		1.9	3.12	6.91	5.81
Space-Time Yield of CH_3OH, (mol/l-cat.hr)		0.3769	1.0833	1.8988	0.9327
Space-Time Yield of DME (mol/l-cat.hr)		-	-	0.1581	0.2720

Reaction Condition P = 20 atg

GHSV = 8000 hr^{-1}

Reaction Temperature (°C)		205	233	267	297
Product Selectivity	CH_3OH (%)	44.44	63.64	12.90	41.66
	CO_2 (%)	16.67	18.18	43.01	25.0
	CH_4 (%)	-	-	-	-
	C_2H_6 (%)	-	-	-	-
	C_3H_8 (%)	-	-	-	-
	C_2H_4 (%)	-	-	-	-
	C_3H_6 (%)	-	-	-	-
	CH_3OCH_3 (%)	-	-	2.15	16.67
	other H.C(%)	38.89	18.18	41.94	16.67
	total H.C(%)	38.89	18.18	41.94	16.67
Conversion of CO (%)		1.06	1.36	9.99	6.0
Space-Time Yield of CH_3OH, (mol/l-cat.hr)		0.5608	1.0304	1.5342	2.9757
Space-Time Yield of DME (mol/l-cat.hr)		-	-	0.1278	0.5954

Reaction Condition P = 20 atg

GHSV = 16000 hr^{-1}

Reaction Temperature (°C)		202	234	264	291
Product Selectivity	CH_3OH (%)	-	57.14	4.90	8.19
	CO_2 (%)	50	21.43	2.45	4.1
	CH_4 (%)	-	-	-	1.29
	C_2H_6 (%)	-	-	-	-
	C_3H_8 (%)	-	-	-	-
	C_2H_4 (%)	-	-	-	-
	C_3H_6 (%)	-	-	-	-
	CH_3OCH_3 (%)	-	-	-	3.28
	other H.C(%)	50	21.43	92.65	83.14
	total H.C(%)	50	21.43	92.65	84.43
Conversion of CO (%)		0.2814	0.7274	9.78	12.28
Space-Time Yield of CH_3OH, (mol/l-cat.hr)		-	0.9896	1.141	2.3946
Space-Time Yield of DME (mol/l-cat.hr)		-	-	-	0.4795

VITA

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