4. PARTICIPATING PROJECT PERSONNEL

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Table 2: Patent [1], CMRU-8, and CMRU-9 Results on K-$Cu_{0.5}Mg_5CeO_x$

	Patent	CMRU-8	CMRU-9
Catalyst	K-$Cu_{0.5}Mg_5CeO_x$	$Cu_{0.5}Mg_5CeO_x$	K-$Cu_{0.5}Mg_5CeO_x$
Mg/Ce	5	5	5
Source		MG3-1b O	MG3-1b O/K
Data File		\1c8-1832.1-9	\1c9-180!.1-9
Charge (g)	3.00	2.98	3.00
T (°C)	320	325	250
P (atm)	50	50	50
GHSV (cm^3(STP)/g cat.h)	1832	1832	1800
H2:CO	1	1	1
CO Conversion	15.5%	5.4%	19.2%
Product Selectivities			
methanol	**57.19**	**87.76**	**96.90**
ethanol	1.87	0.73	0.42
1-propanol	2.64	0	0.12
isopropanol	not reported	0	0
2-butanol	not reported	0	0.07
isobutanol	**10.44**	0	**0.21**
1-butanol	0.28	0	0
1-pentanol	0.68	0	0
2-methyl-1-butanol	1.17	0	0
paraffins	24.31	11.17	2.05
CO2	31.04	15.43	3.55
Σ Selectivities-Sel. CO_2	105	100	100

Table 3: Patent [1] and CMRU-10 Results on K-$Cu_{0.5}Mg_5CeO_x$

	Patent	**CMRU-10**	**CMRU-10**
Catalyst	0.9% K - $Cu_{0.5}Mg_5CeO_x$	3.0% K - $Cu_{0.5}Mg_5CeO_x$	3.0% K - $Cu_{0.5}Mg_5CeO_x$
Mg/Ce	5	5	5
Source		MG3-1b O/K	MG3-1b O/K
Data File		\1cmru-10.4-12	\2cmru-10.1-7
Charge (g)	3.00	3.04	3.04
T (°C)	320	250	250
P (atm)	50	50	50
GHSV (cm^3(STP)/g cat.h)	1832	1776	888
H2:CO	1	1	1
CO Conversion	15.5%	3.3%	6.5%
Product Selectivities			
methanol	**57.19**	**97.5**	**93.2**
ethanol	1.87	0.93	0.69
1-propanol	2.64	0.06	0.22
1-butanol	0.28	0	0
isobutanol	**10.44**	**0.10**	**0.37**
1-pentanol	0.68	0	0
2-methyl-1-butanol	1.17	0	0
paraffins	24.31	1.31	5.13
CO2	31.04	14.52	8.34
Σ Selectivities-Sel. CO_2	105	100	100

Table 4: Patent [1], CMRU-12, and CMRU-13 Results at T = 320 °C

	Patent	CMRU-12	CMRU-13
Catalyst	0.9% K - $Cu_{0.5}Mg_5CeO_x$	0.9% K - $Cu_{0.5}Mg_5CeO_x$	0.9% K - $Cu_{0.5}Mg_5CeO_x$
BET S.A. (m2/g)	not reported	162	190
Mg/Ce	5	5	5
Source		MG3-10b O/K	MG3-10 O/K
		\3cmru12.1-9	\3cmru13.12-9
Charge (g)	3.00	3.01	4.32
T (°C)	320	320	321
P (atm)	50	50	50
GHSV (cm^3(STP)/g cat.h)	1832	1794	1813
H2:CO	1	1	1
CO Conversion	15.5%	14.4%	20.8%
Product Selectivities			
methanol	**57.19**	**73.72**	**65.05**
ethanol	1.87	0.30	0.36
1-propanol	2.64	0.49	2.95
isopropanol	not reported	0.82	0.98
2-butanol	not reported	0.45	0.23
isobutanol	**10.44**	**7.85**	**12.96**
1-butanol	0.28	0.01	0.32
1-pentanol	0.68	0.13	0.16
2-methyl-1-butanol	1.17	0.51	1.04
CO2	31.04	25.85	12.29
DME	1.16	1.86	1.33
acetaldehyde	not reported	not detected	0.24
CH4	**11.52**	**6.86**	**3.68**
C2+ paraffins	12.79	2.67	0.52
MeOH/i-BuOH	5.5	9.4	5.0
Alc/HCs	2.94	9.26	22.7

Table 5: Patent [1], CMRU-12, and CMRU-13 Results at T > 330 °C

	Patent	CMRU-12	CMRU-12	CMRU-13
Catalyst	0.9% K - $Cu_{0.5}Mg_5CeO_x$	0.9% K - $Cu_{0.5}Mg_5CeO_x$	0.9% K - $Cu_{0.5}Mg_5CeO_x$	0.9% K - $Cu_{0.5}Mg_5CeO_x$
BET S.A. (m^2/g)	not reported	162	162	190
Mg/Ce	5	5	5	5
Source		MG3-10b O/K	MG3-10b O/K	MG3-10 O/K
		\4cmru12	\6cmru12	\4cmru13b
Charge (g)	3.00	3.01	3.01	4.32
T (°C)	**360**	**341**	**362**	**331**
P (atm)	50	50	50	50
GHSV (cm^3(STP)/g cat.h)	1832	1794	1794	1813
H2:CO	1	1	1	1
CO Conversion	19.0%	8.0%	4.1%	6.8%
Product Selectivities				
methanol	26.27	72.44	57.08	41.47
isobutanol	10.94	14.80	17.40	26.65
paraffins	60.1	4.07	10.58	6.16
CO_2	not reported	29.44	54.62	23.69
Σ Selectivities-Sel. to CO_2	100	100	100	100
MeOH/i-BuOH	2.4	5.0	3.3	1.6
Alc/HCs	0.66	26.2	7.8	14.7

Table 6: CMRU-13 (MG3-10 O/K) and CMRU-14 (MG3-10 O/Cs) Results

	CMRU-13	CMRU-14
Catalyst	0.9% K-$Cu_{0.5}Mg_5CeO_x$	0.9% Cs-$Cu_{0.5}Mg_5CeO_x$
BET S.A. (m^2/g)	190	143
Mg toCe ratio	5	5
Source	MG3-10 O/K	MG3-10 O/Cs
	\3cmru13.12-9	\4cmru14.1-9
Charge (g)	4.32	3.21
T (°C)	321	320
P (atm)	50	50
GHSV (cm^3/g cat.h)	1813	1862
H2:CO	1	1
CO Conversion	20.8%	9.0%
Product Selectivities		
methanol	**65.05**	**62.12**
ethanol	0.36	1.11
1-propanol	2.95	5.02
isopropanol	0.98	2.99
2-butanol	0.23	0.32
isobutanol	**12.96**	**11.58**
1-butanol	0.32	0.12
1-pentanol	0.16	0.56
2-methyl-1-butanol	1.04	1.39
CO2	12.29	22.39
DME	1.33	2.44
acetaldehyde	0.24	0.43
CH4	3.68	2.33
C2+ paraffins	0.52	0.28
Σ Selectivities-Sel. to CO_2	100	100
MeOH/i-BuOH	5.0	5.4
Alc/HCs	22.7	31.9

Table 9: CMRU-15 (MG3-11 O/K) and CMRU-16 (MG3-11 O) Results

	CMRU-15	CMRU-16
Catalyst	0.9% K - $Cu_{0.5}Mg_5CeO_x$	$Cu_{0.5}Mg_5CeO_x$
BET S.A. (m^2/g)	56	93
Mg toCe ratio	5	5
Source	MG3-11 O/K	MG3-11 O
	\1gc	\1gc8co2
Charge (g)	2.95	3.21
T (°C)	593	593
P (atm)	44	44
GHSV (cm^3(STP)/g cat.h)	6100	5000
H2:CO	1	1
CO Conversion	2.3%	3.2%
Product Selectivities		
methanol	**67.78**	**80.07**
ethanol	3.56	1.91
1-propanol	3.11	2.00
isopropanol	0.93	0.53
2-butanol	0.52	0
isobutanol	**10.22**	**2.77**
1-butanol	0.00	0.31
1-pentanol	0.00	0.11
2-methyl-1-butanol	0.12	0
CO2	16.92	8.70
DME	1.85	1.16
acetaldehyde	0.05	0
CH4	3.35	3.68
C2+ paraffins	0.48	0.78
Σ Selectivities-Sel. to CO_2	100	100
MeOH/i-BuOH	8.5	29.1
Alc/HCs	10.8	20.2

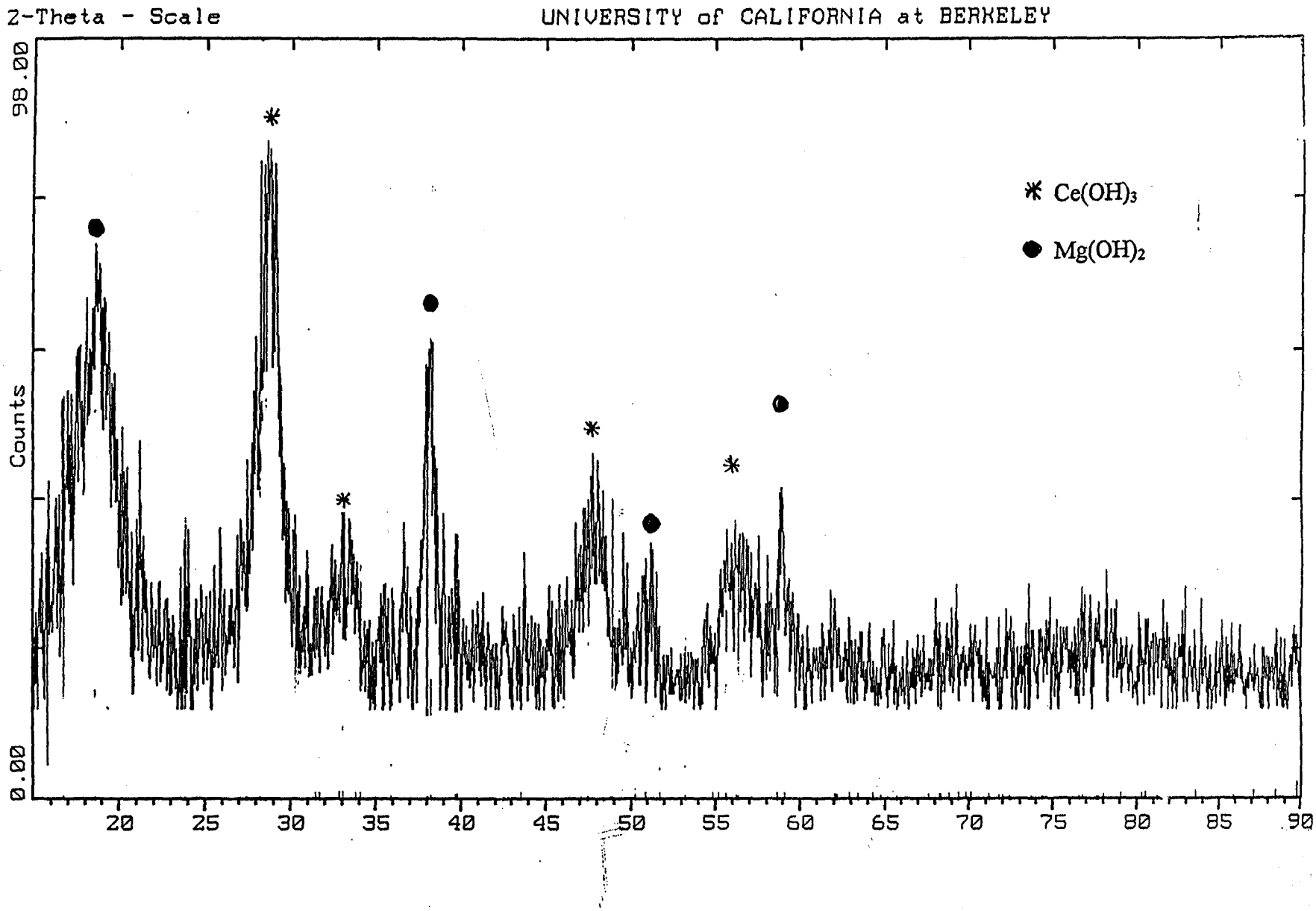


Figure 1: XRD pattern of Cu/Mg/Ce oxide precursor.

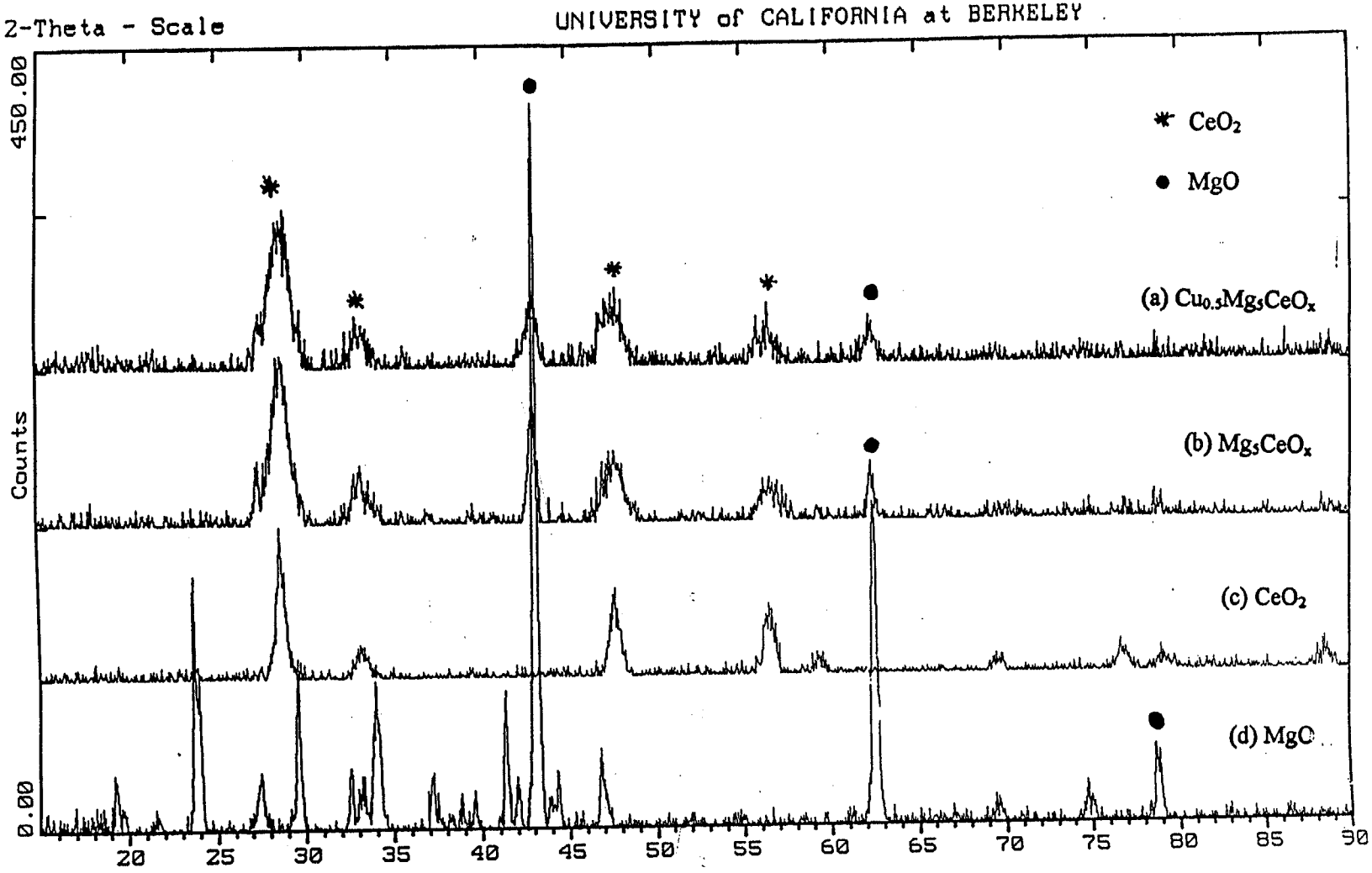


Figure 2: XRD patterns of Cu/Mg/Ce mixed oxides.

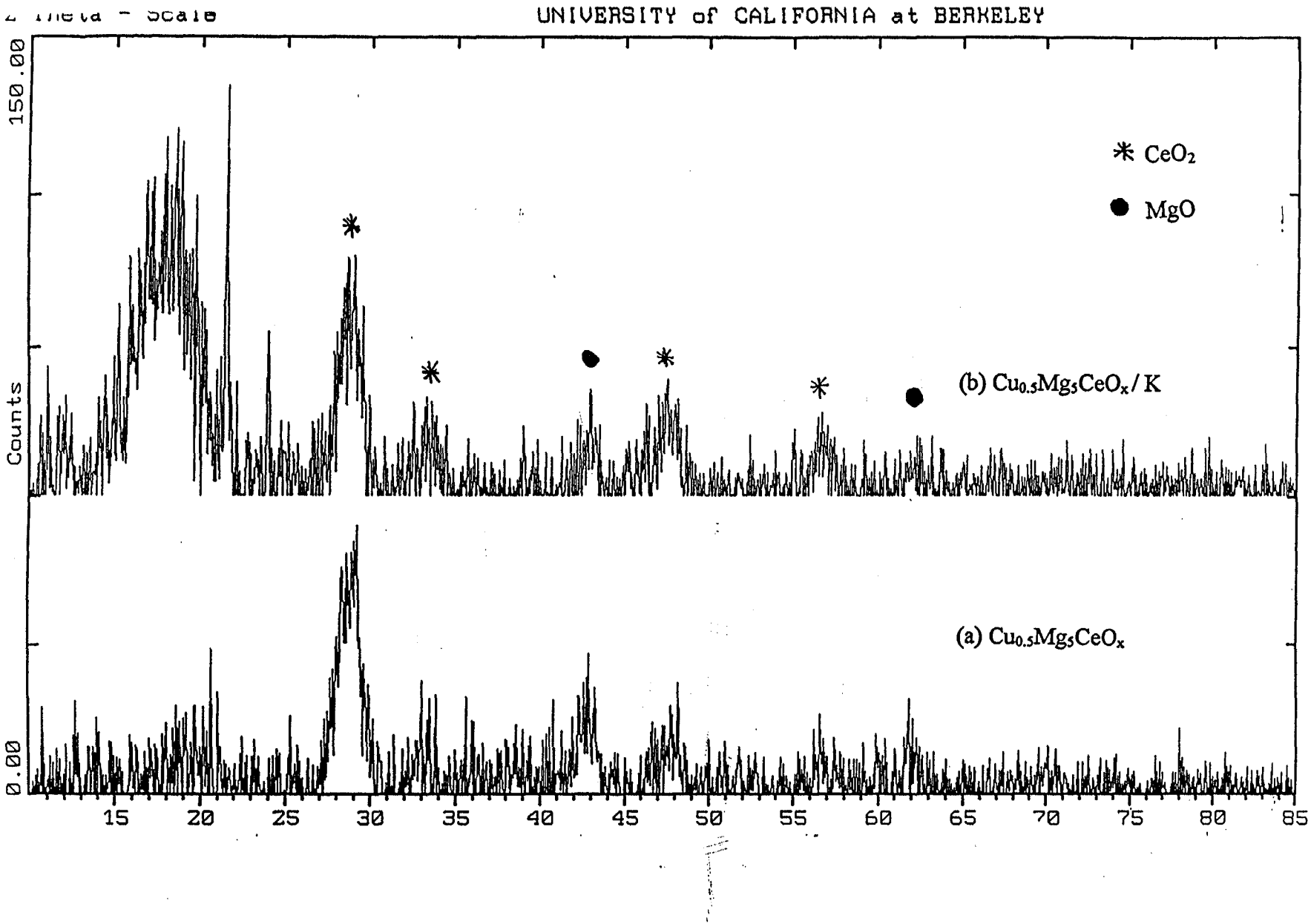


Figure3: XRD pattern of Cu/Mg/Ce oxides. *(a)* Unpromoted catalyst, and *(b)* potassium promoted catalyst.

Fig. 4. Methanol and ethanol turnovers as a function of contact time on Cu/ZnO

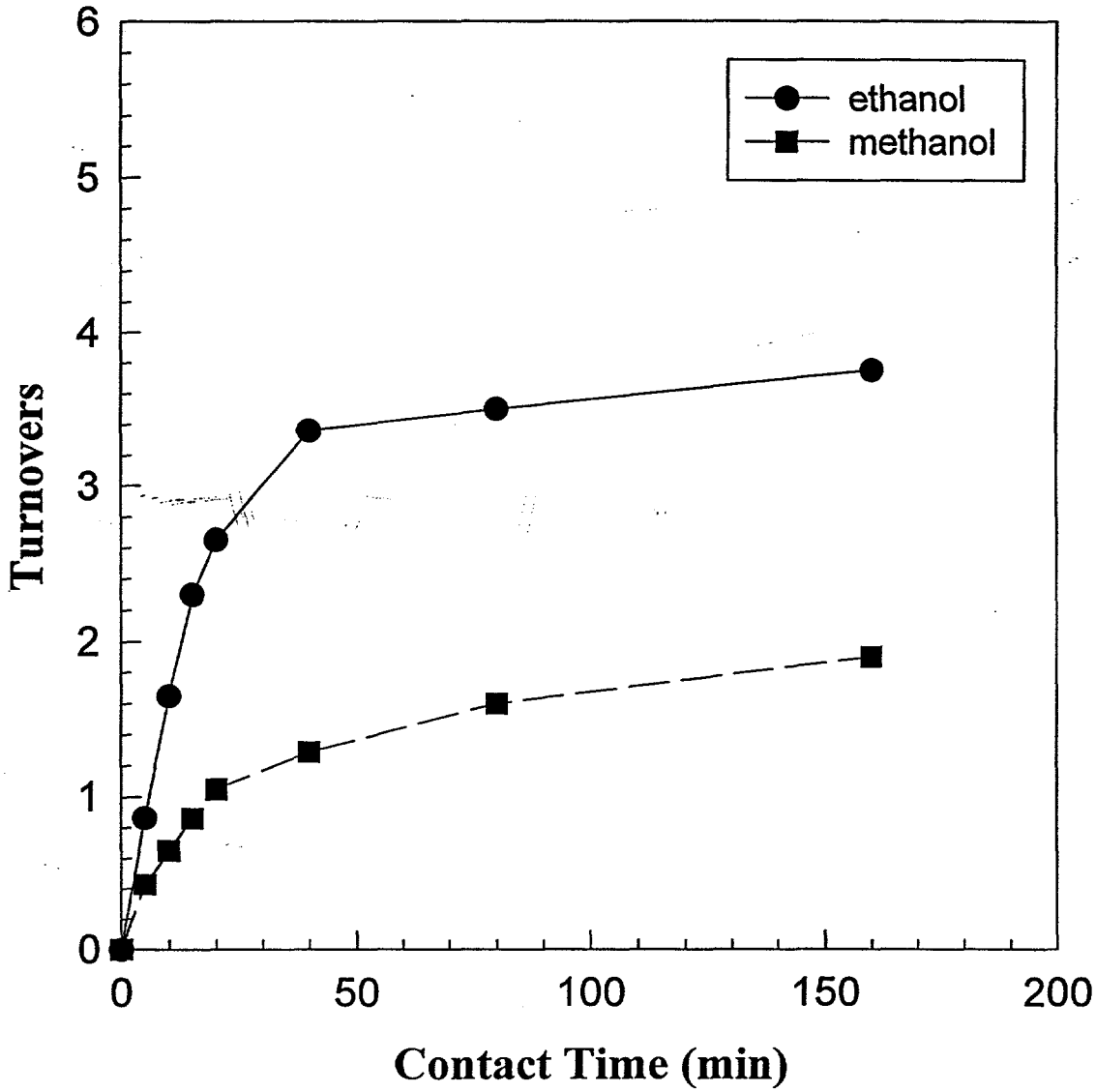


Fig. 5. Product selectivity with respect to ethanol conversion on Cu/ZnO

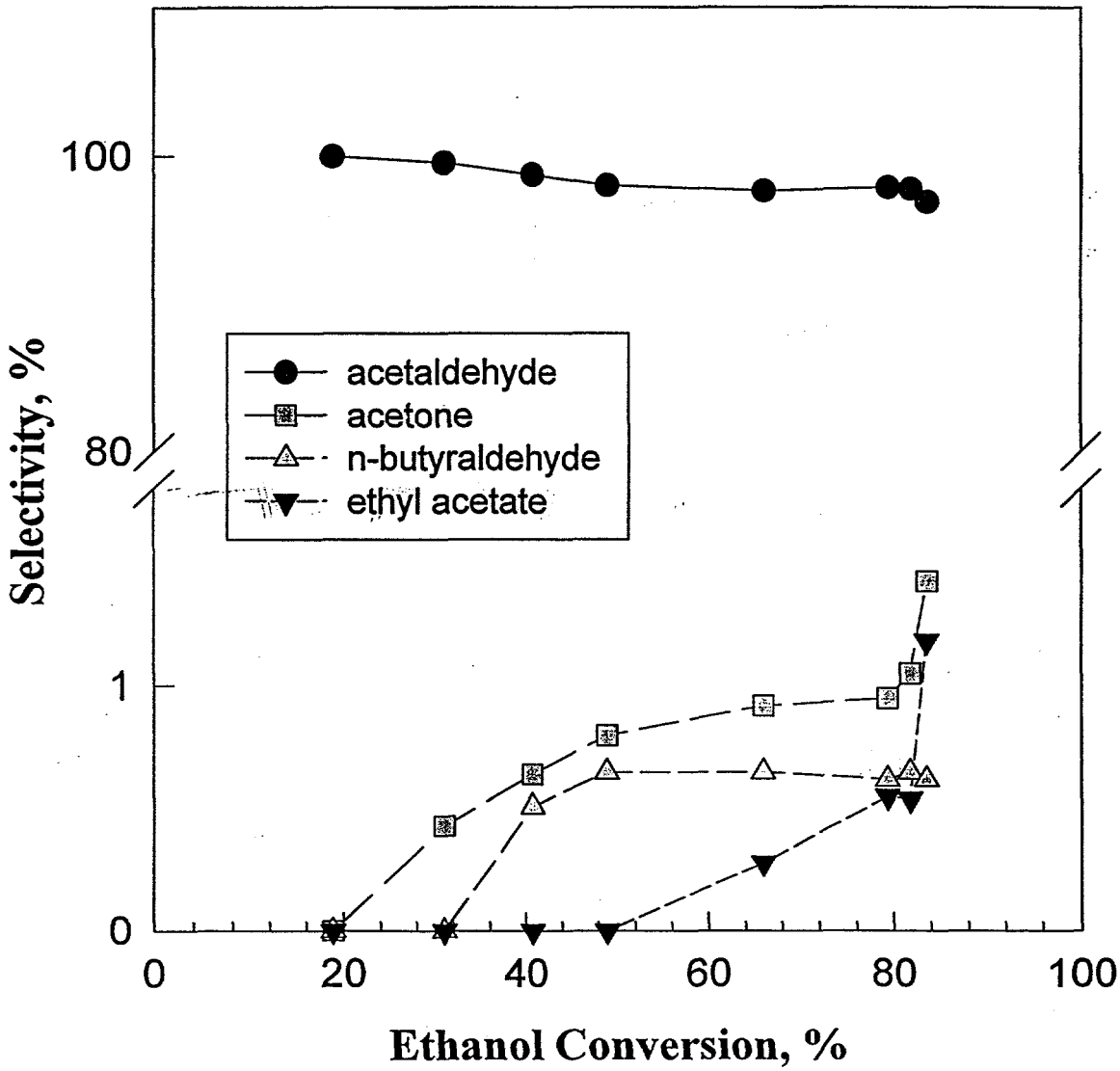


Fig. 6. Ethanol turnovers as a function of time on Cu/ZnO

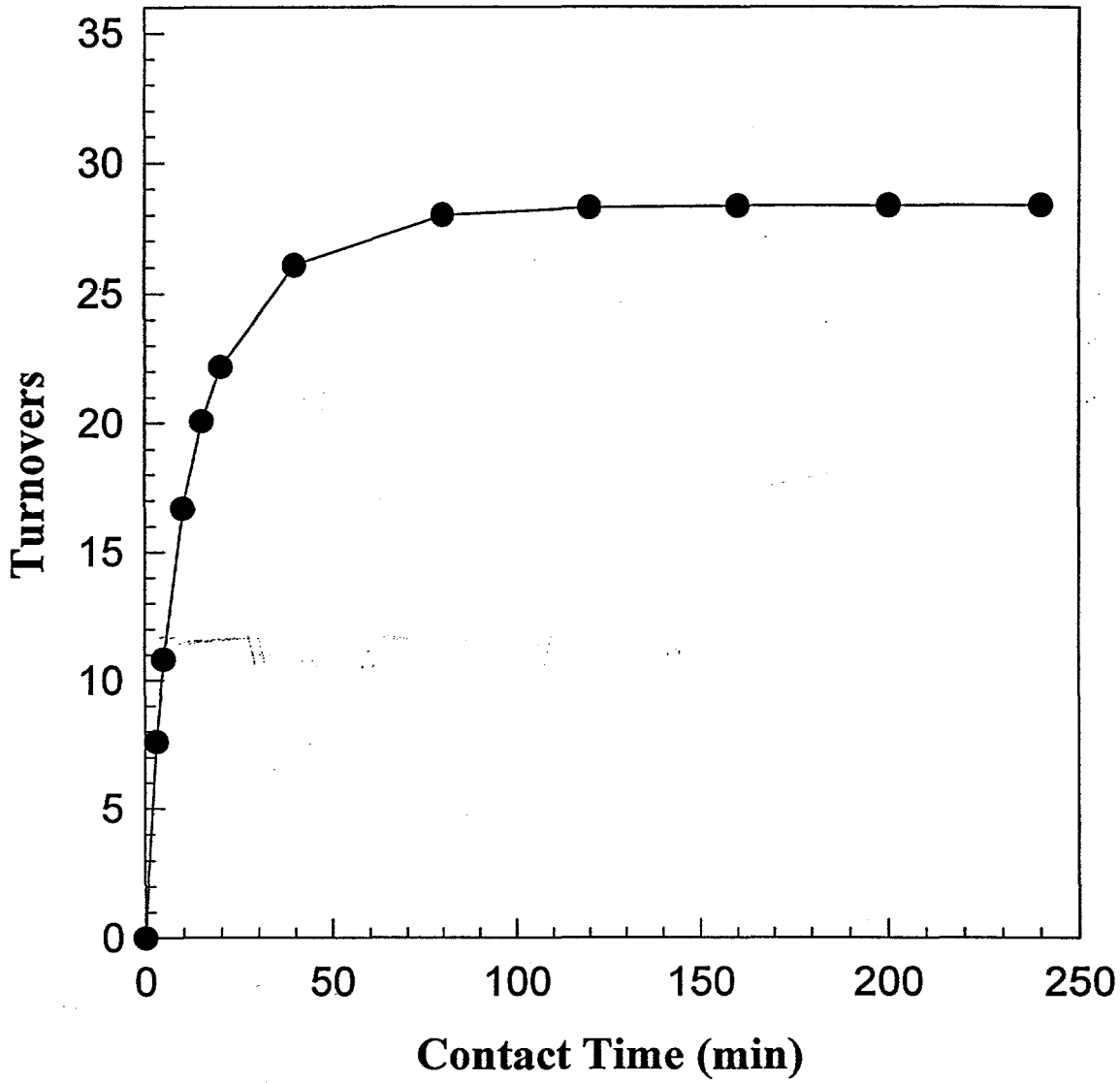


Fig. 7. products selectivity as a function of contact time on Cu/ZnO

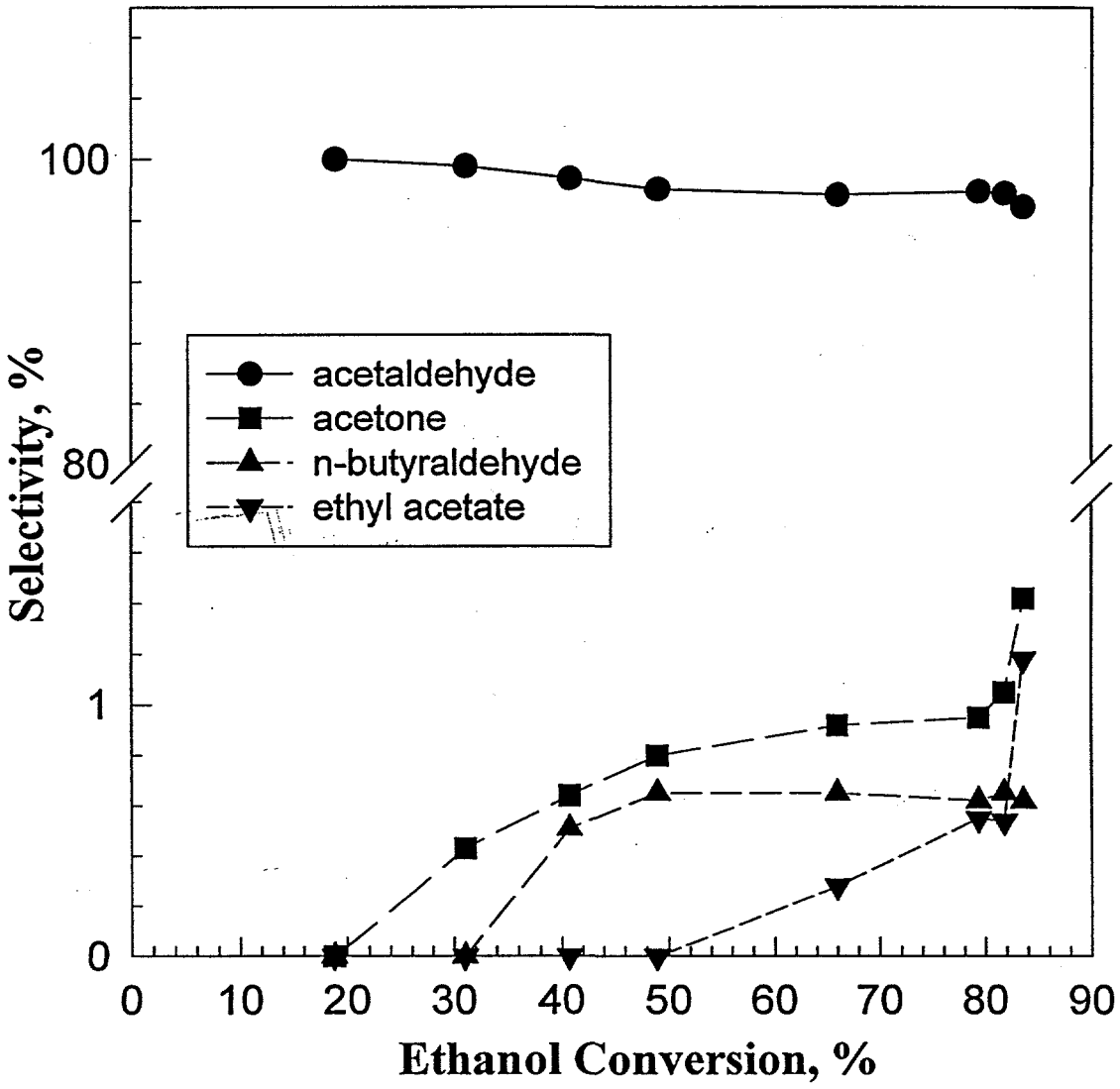


Fig. 8. Ethanol conversion as a function of contact time on Mg_5CeO_x

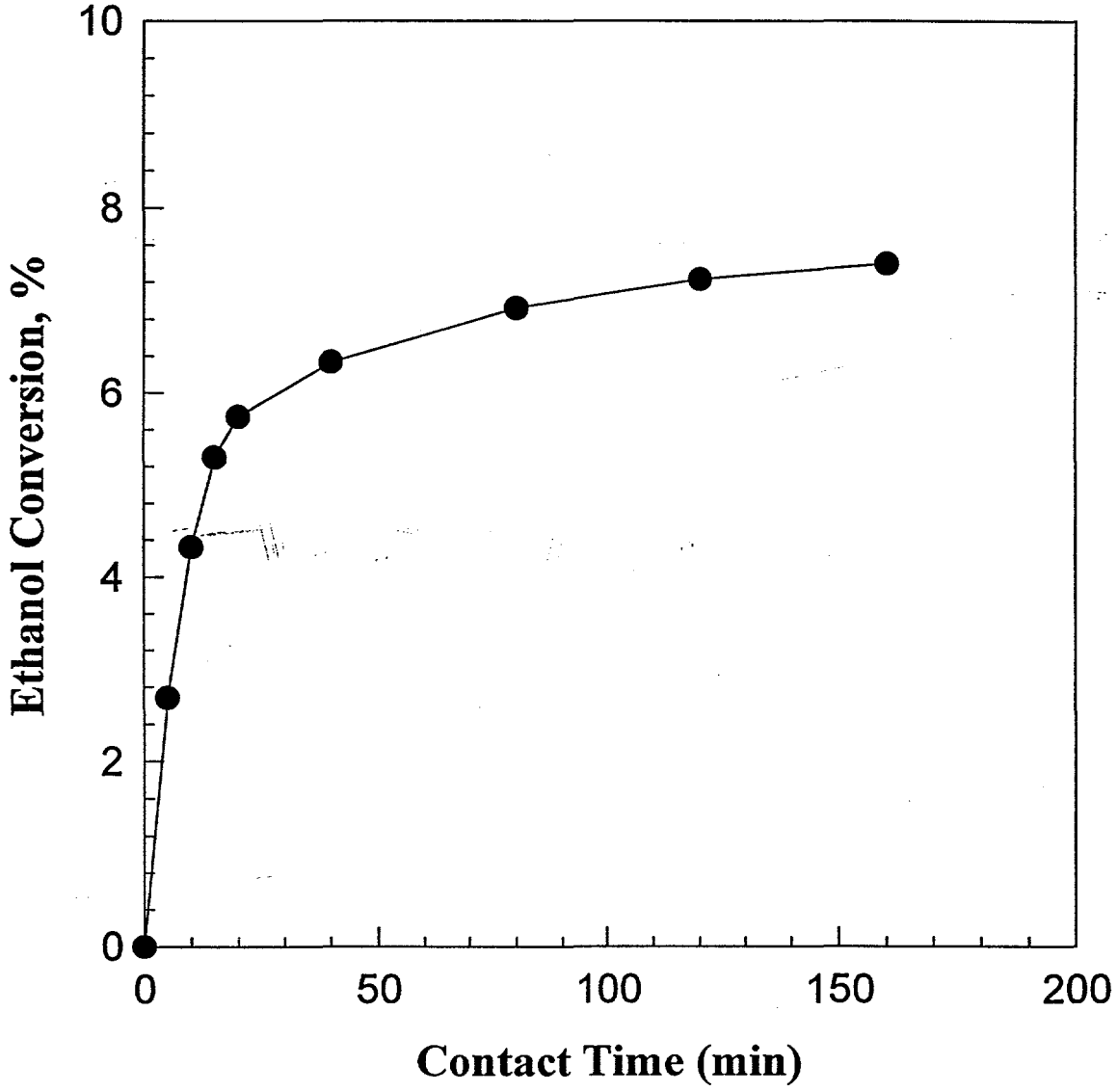


Fig. 9. products distribution as a function of time on Mg_5CeO_x.

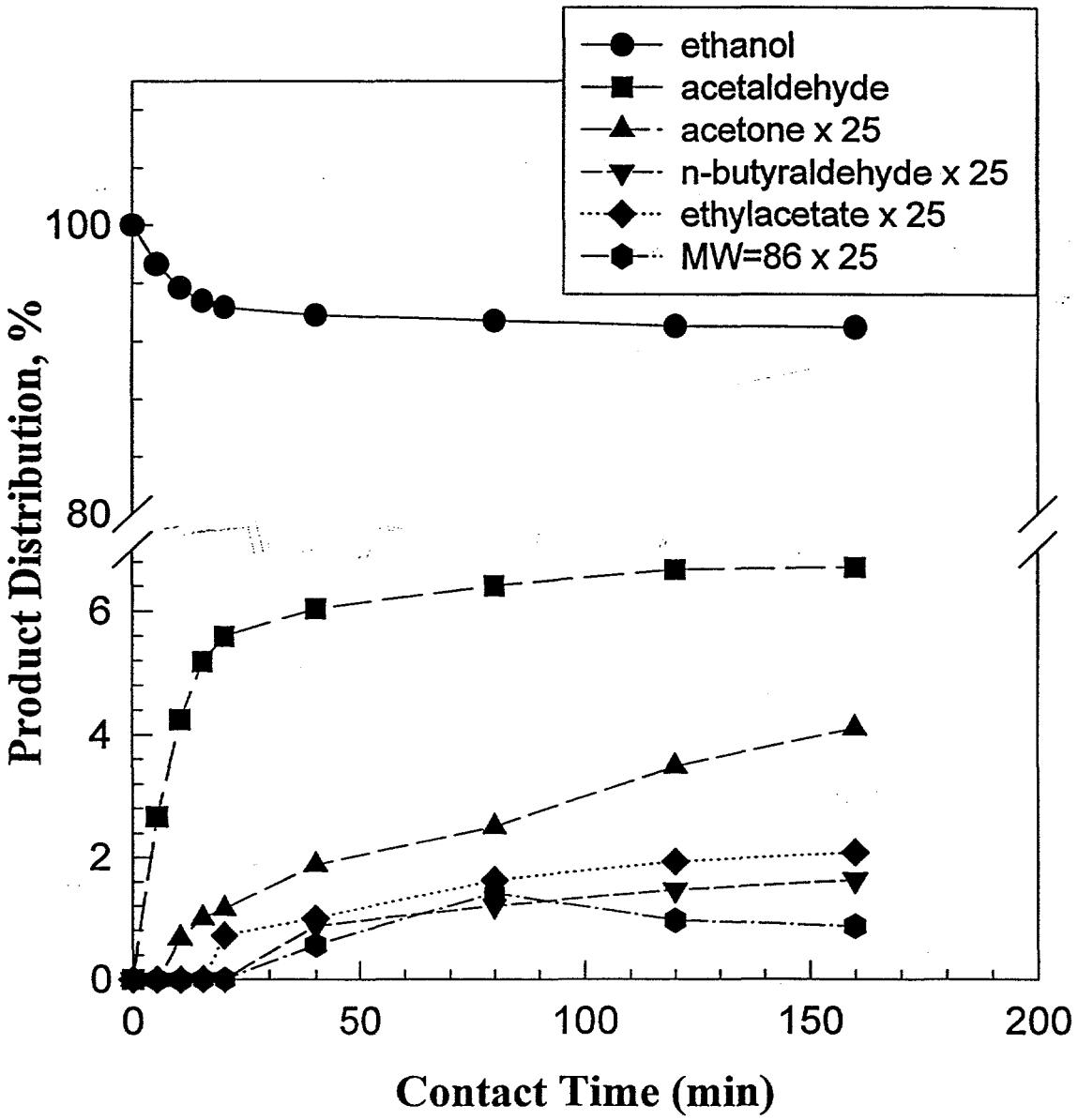


Fig. 10. Ethanol turnovers as a function of time on $Cu_{0.5}Mg_5CeO_x$

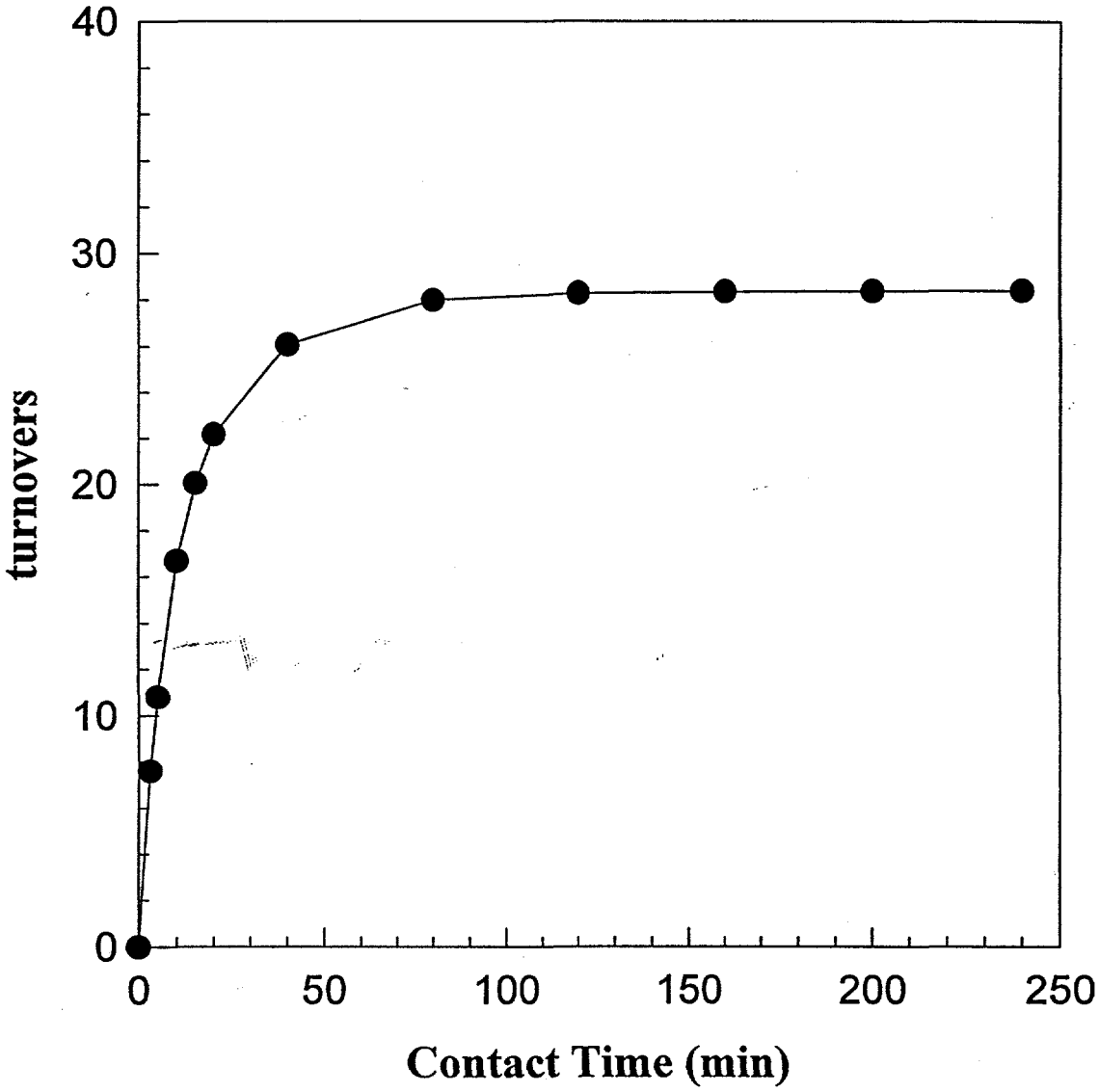


Fig. 11. Ethanol turnovers as a function of time on $Cu_{0.5}Mg_5CeO_X/K$ (1 wt %)

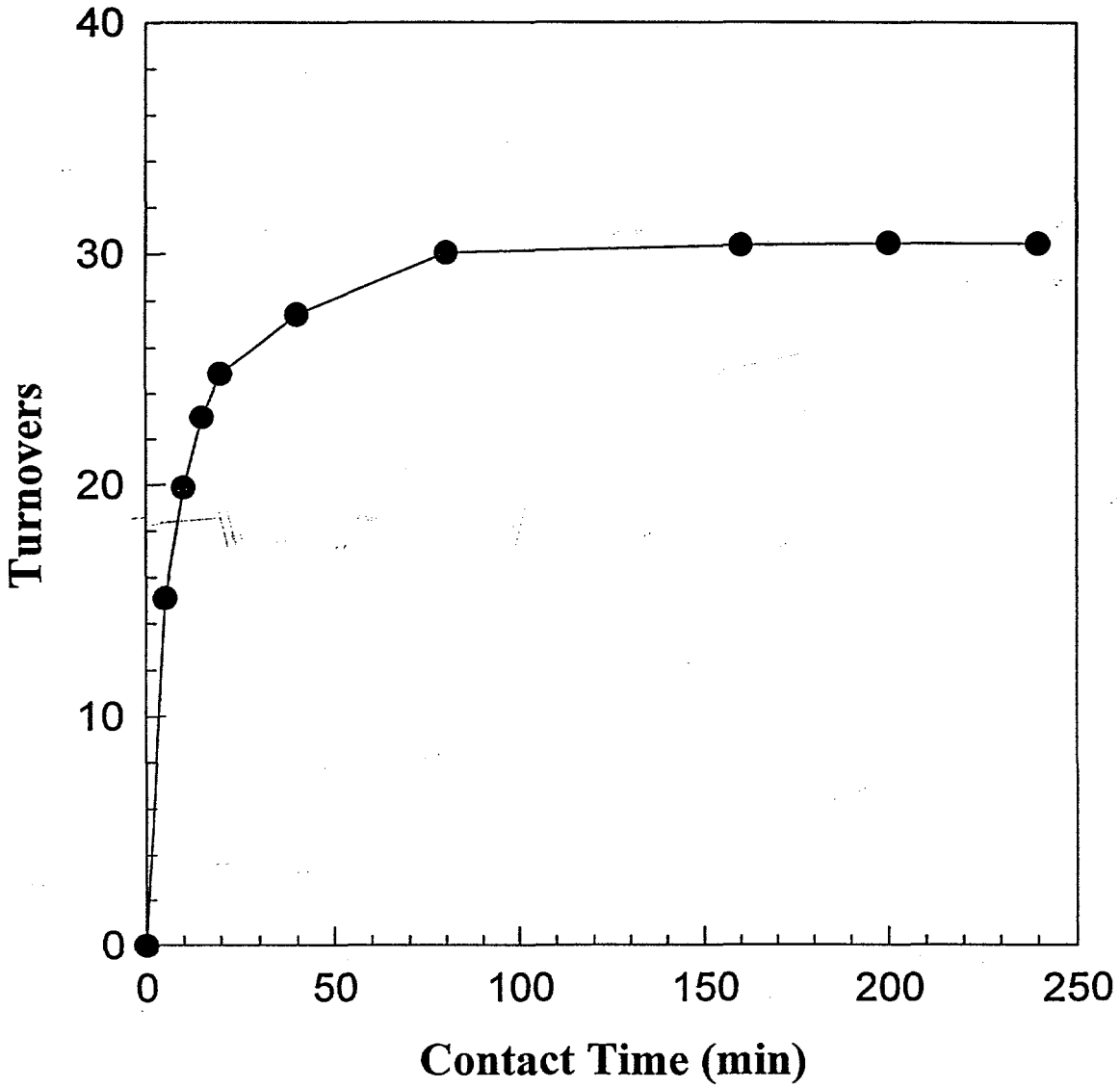


Fig. 12. Product selectivity vs. ethanol conversion$Cu_{0.5}Mg_5CeO_x$

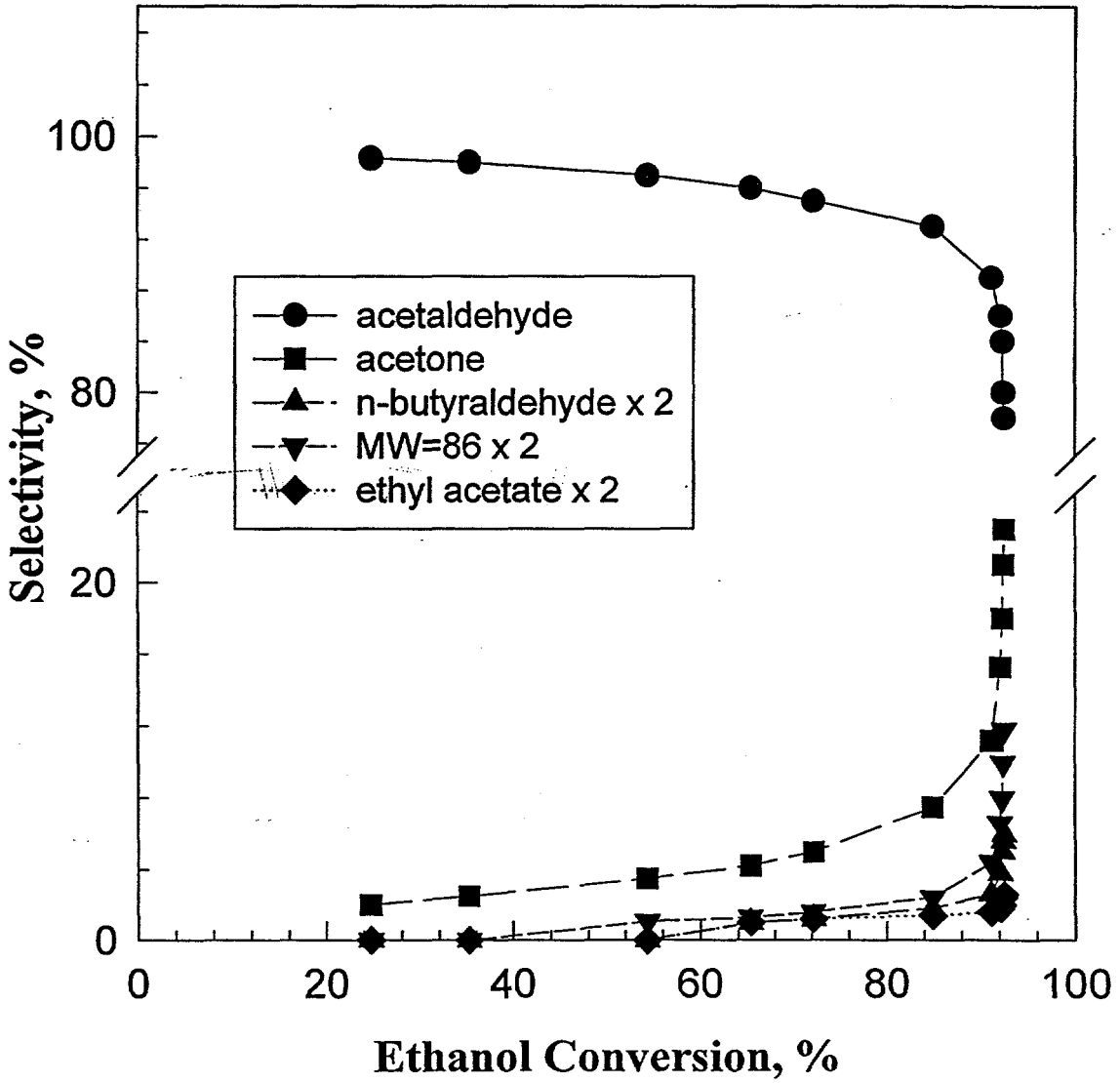


Fig. 13. Product selectivity vs. ethanol conversion on $Cu_{0.5}Mg_5CeO_x/K$ (1 wt %)

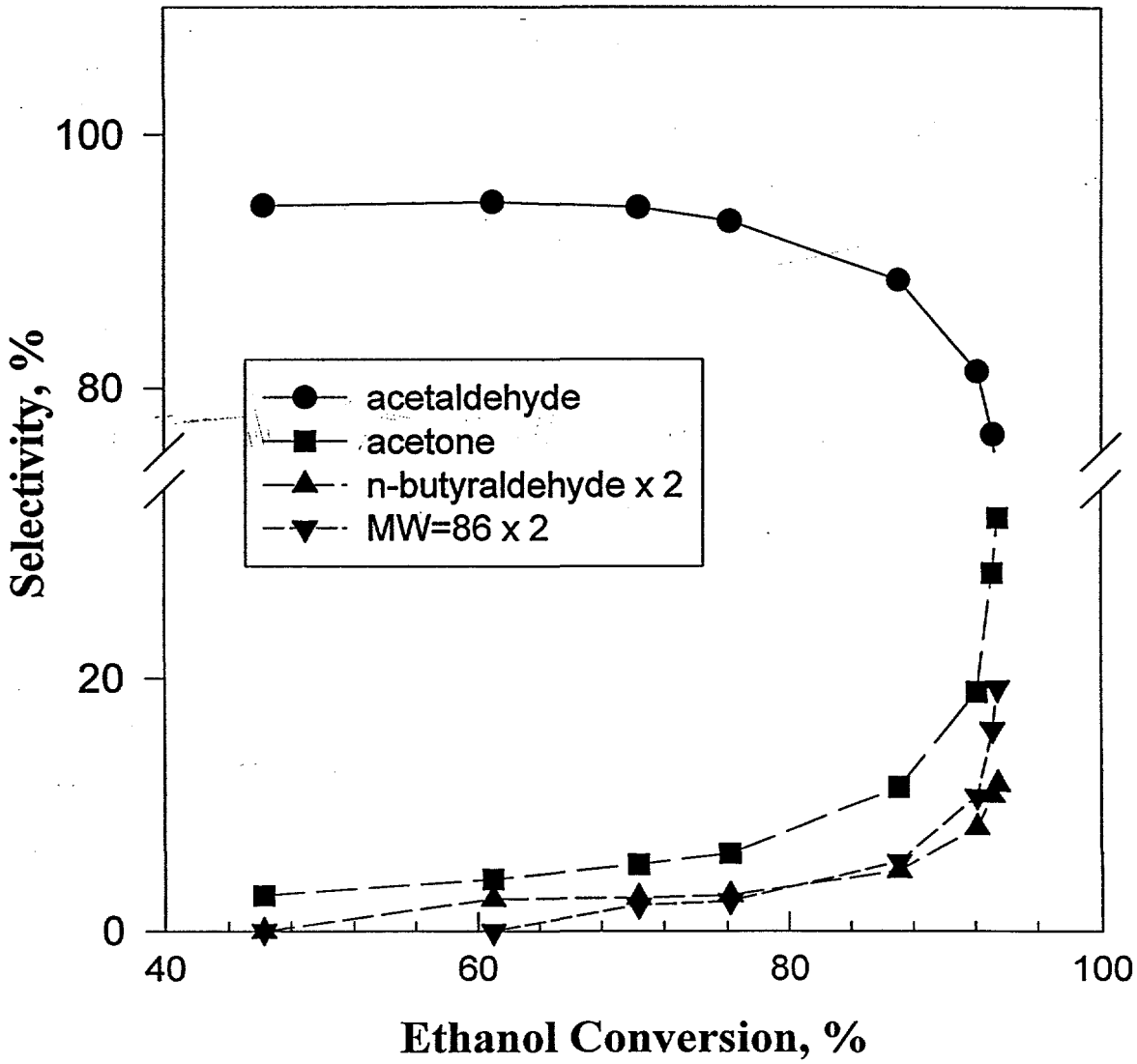


Fig. 14. Products distribution as a function of time on $Cu_{0.5}Mg_5CeO_x$

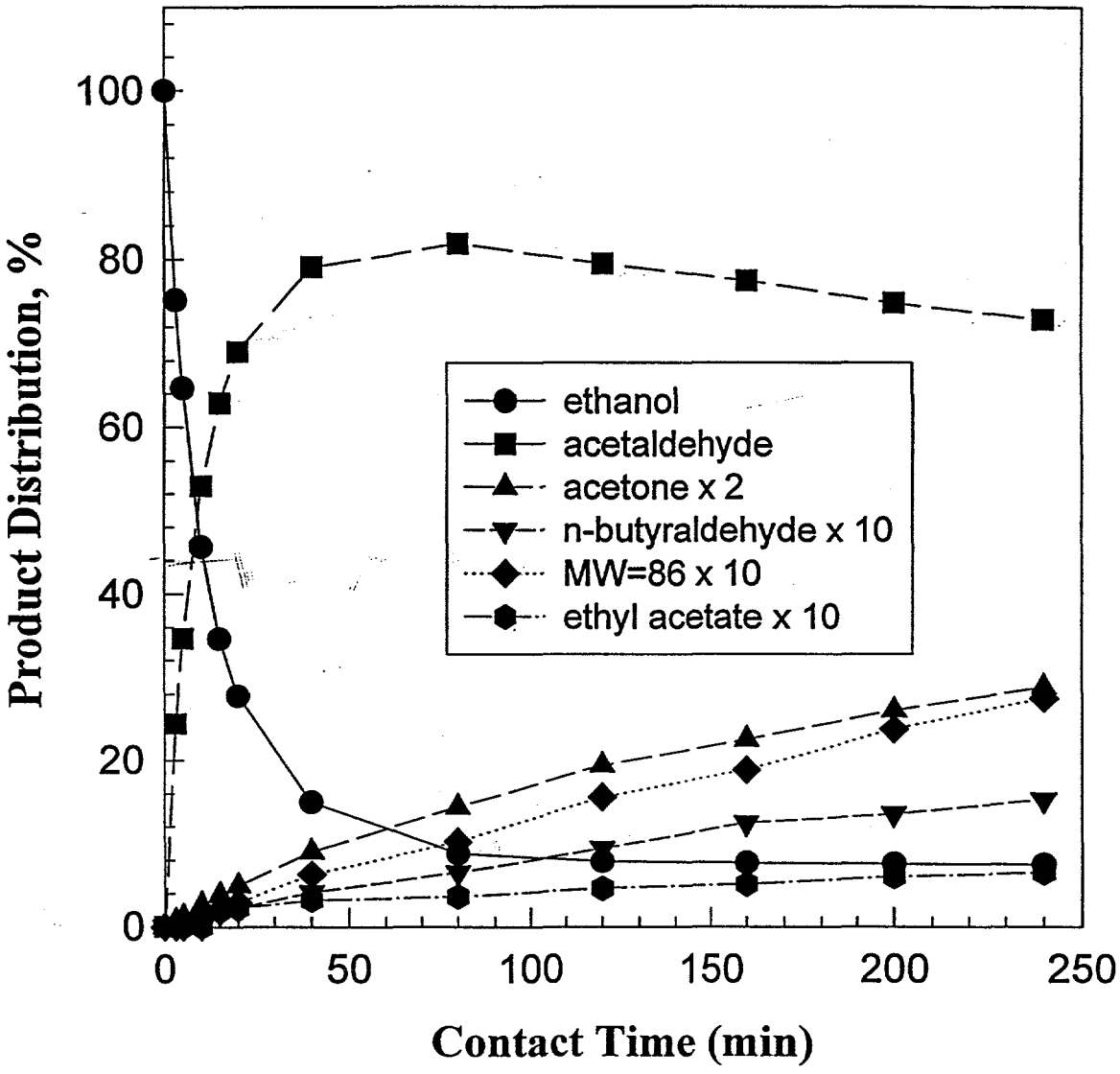


Fig. 15. Product distribution as a function of time on $Cu_{0.5}Mg_5CeO_x/K$ (1wt %)

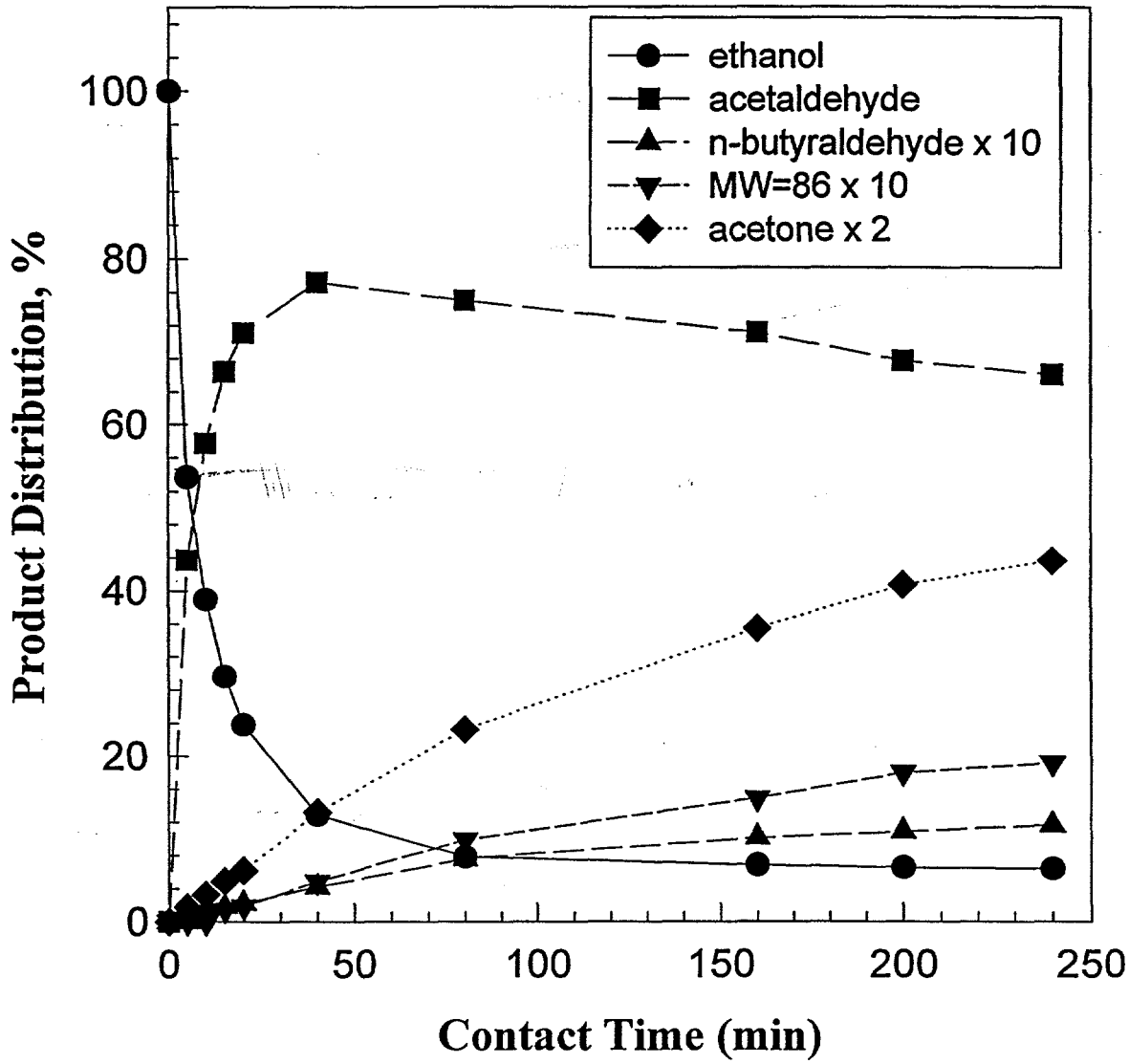
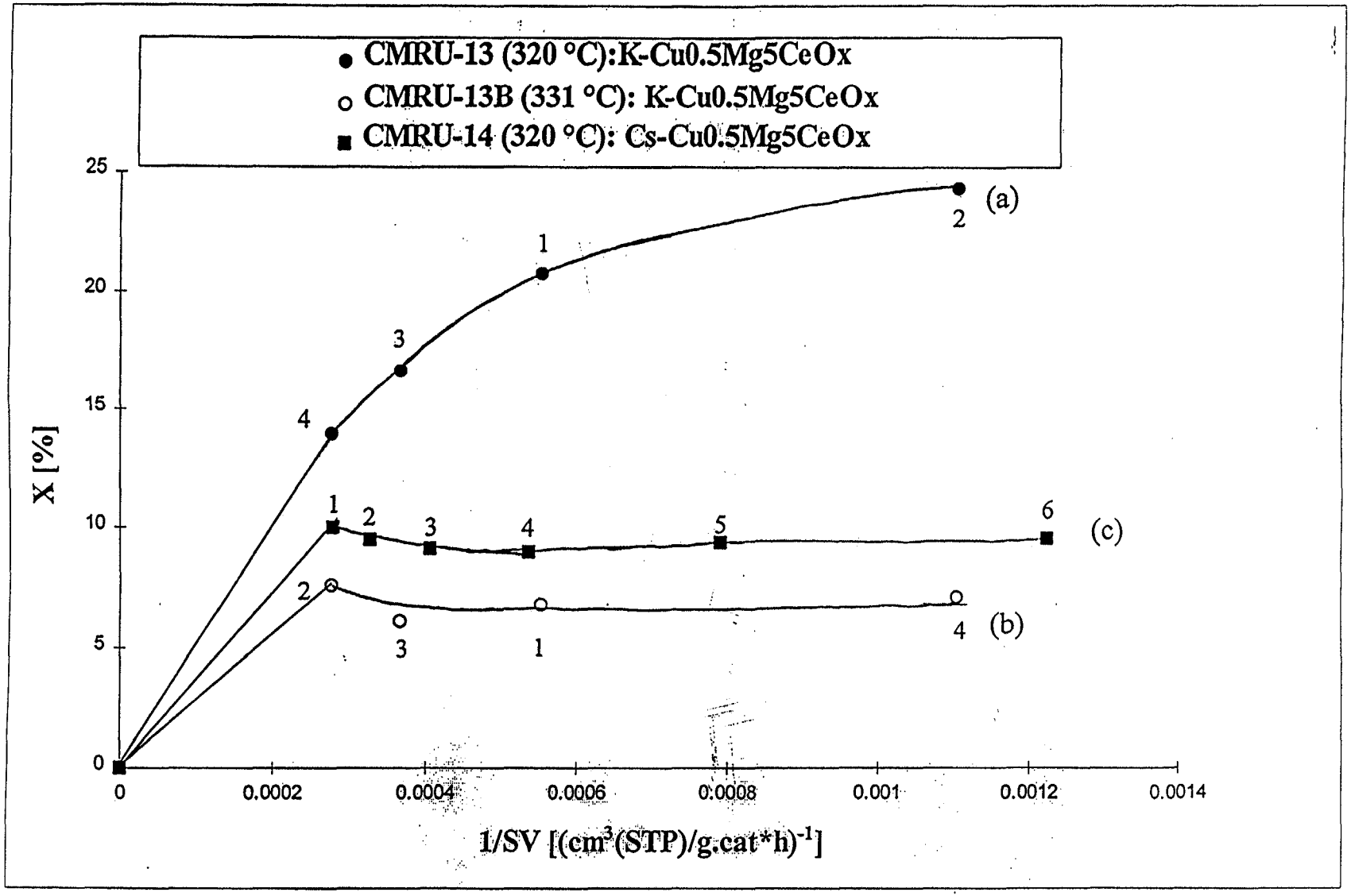


Fig. 16. CO Conversion vs. Reciprocal Space Velocity

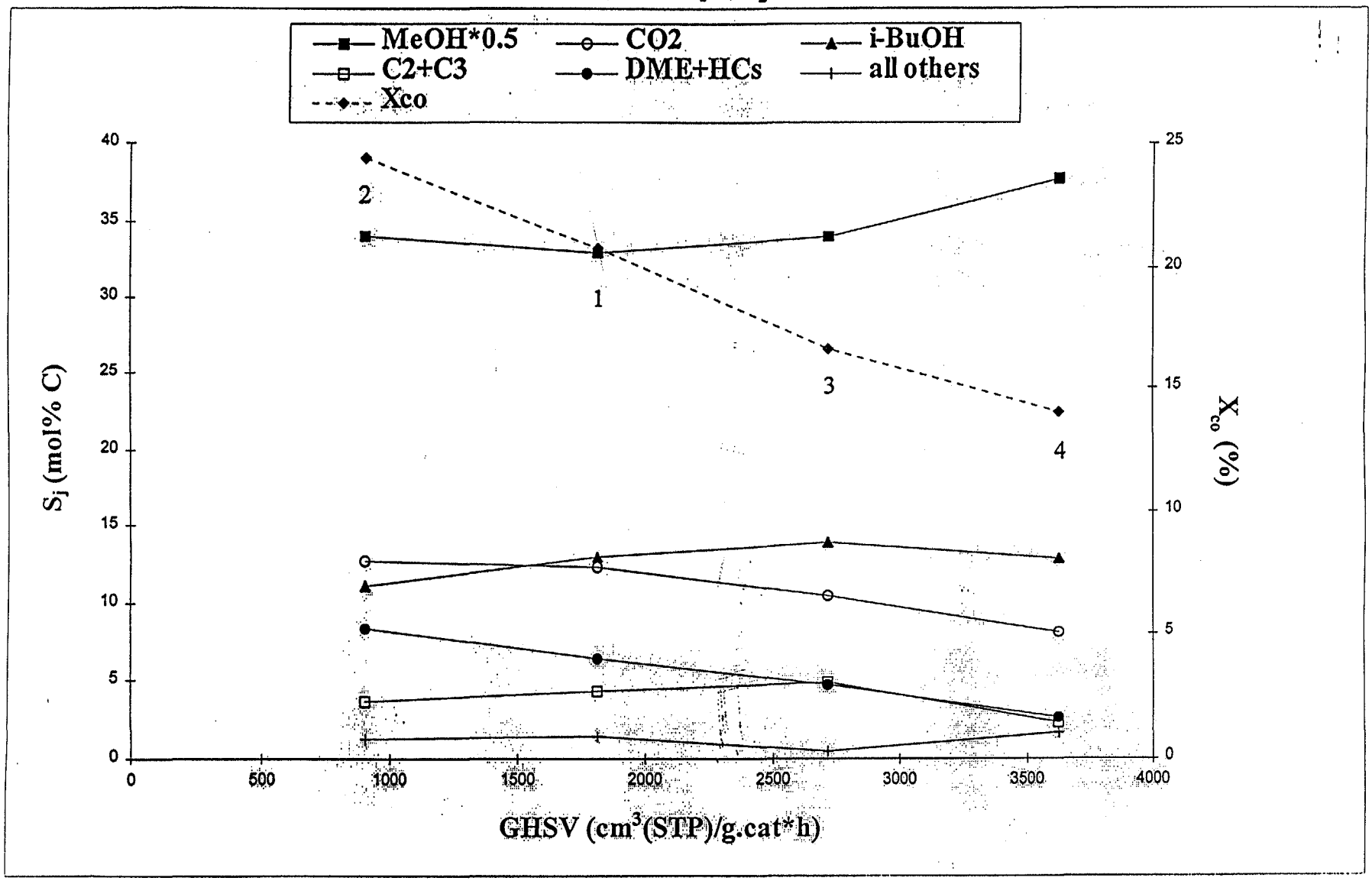


Numbers on plot denote order in which experiment was performed

Fig. 17. Product Selectivities vs. Space Velocity

CMRU-13: K-$Cu_{0.5}Mg_5CeO_x$ (MG3-10 O/K)

T = 320 °C, P = 750 psi, H_2/CO = 1

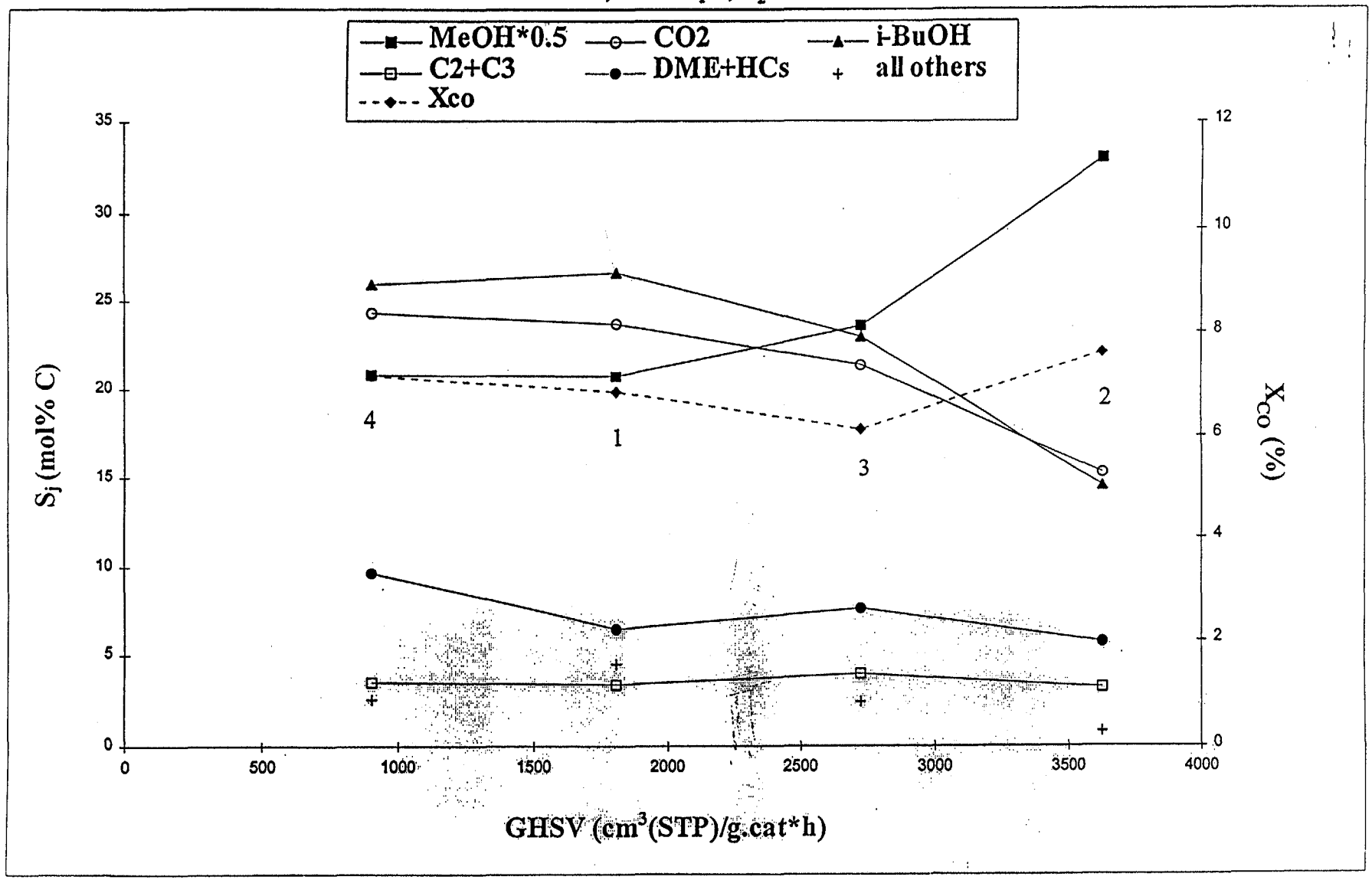


1,2,3,4 denote order in which experiment was performed

Fig. 18. **Product Selectivities vs. Space Velocity**

CMRU-13B: K-$Cu_{0.5}Mg_5CeO_x$ (MG3-10 O/K)

T = 331 °C, P = 750 psi, H_2/CO = 1

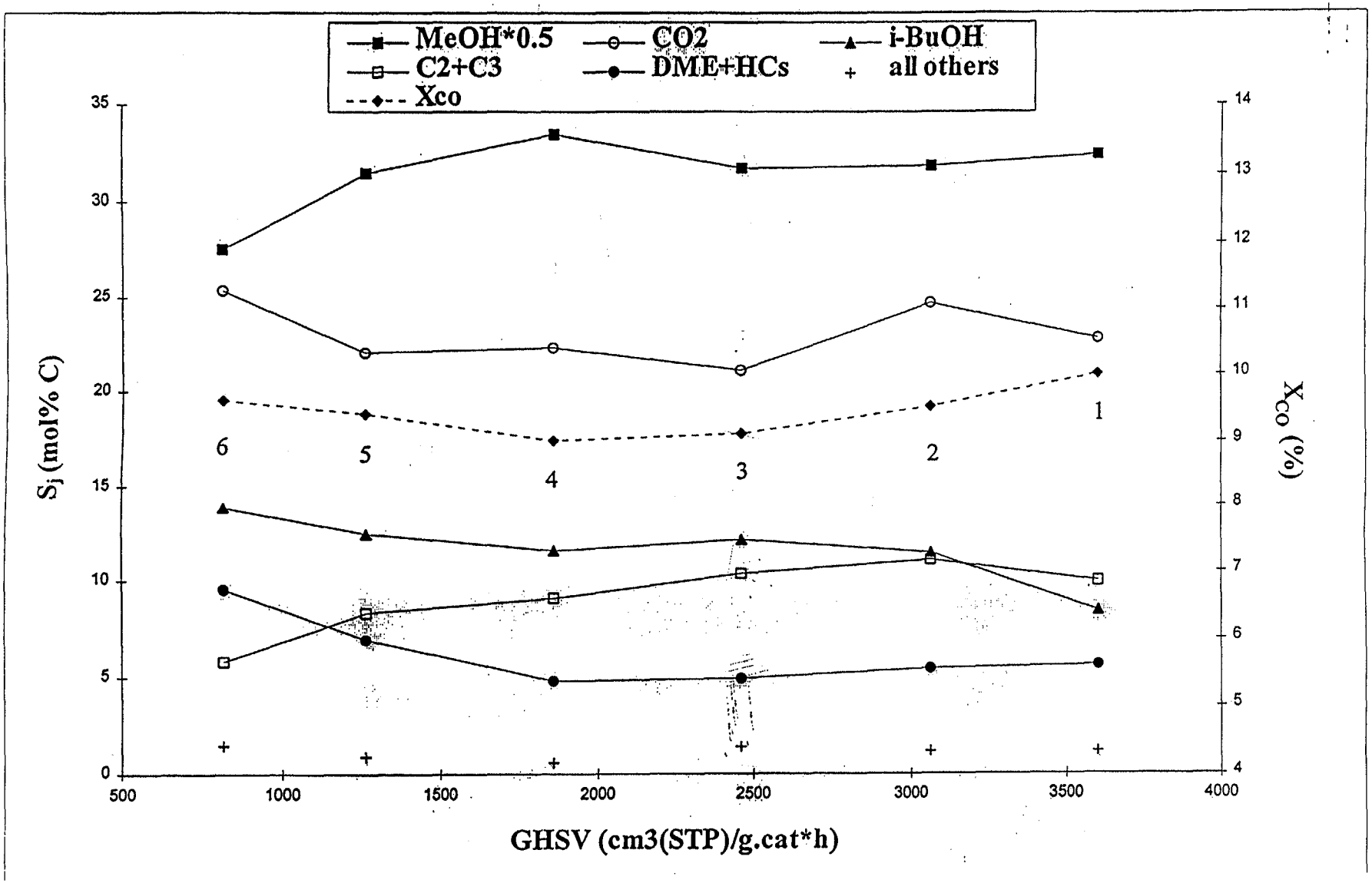


1,2,3,4 denote order in which experiment was performed

Fig. 19. Product Selectivities vs. Space Velocity

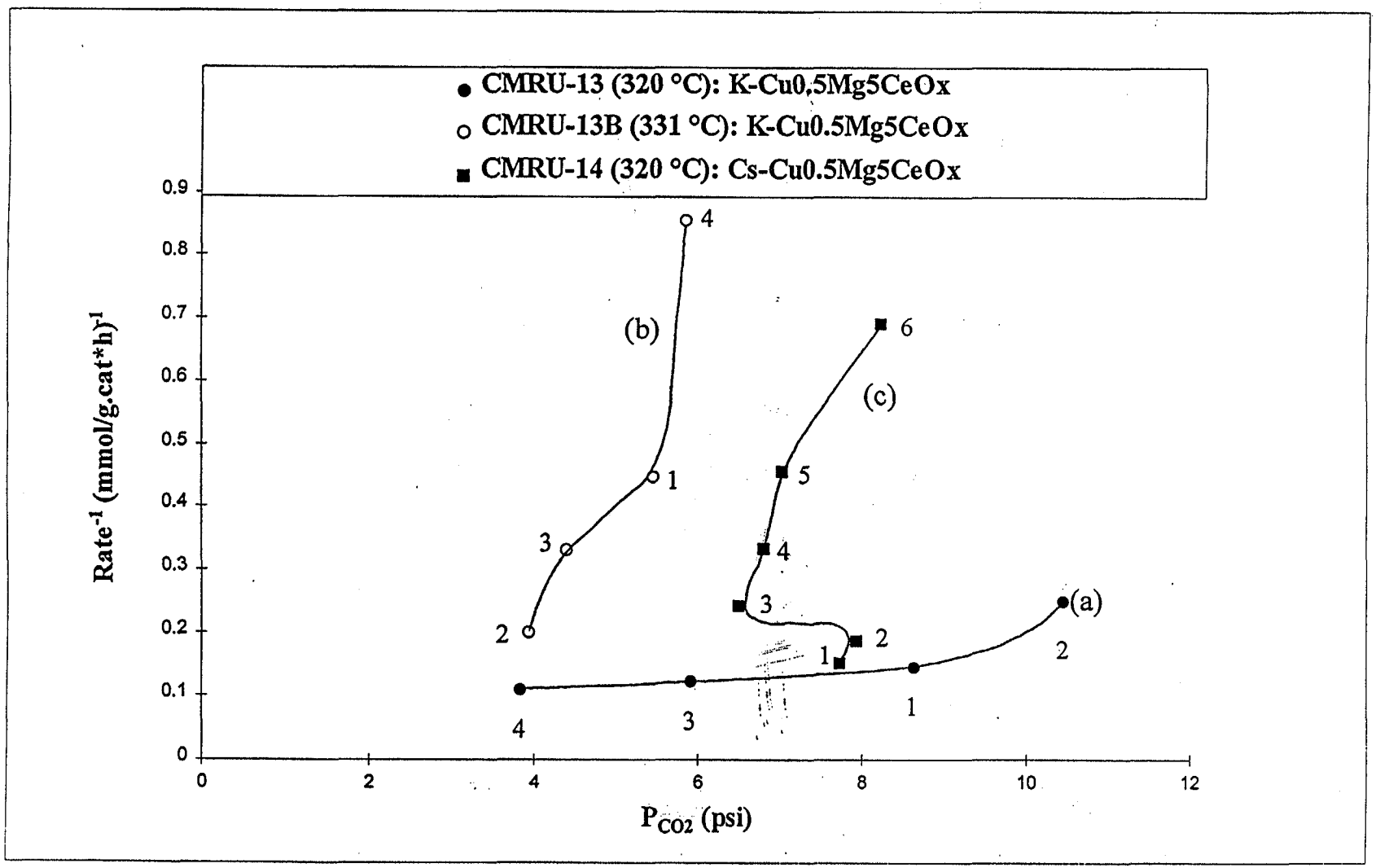
CMRU-14: $Cs\text{-}Cu_{0.5}Mg_5CeO_x$ (MG3-10 O/Cs)

T = 331 °C, P = 750 psi, $H_2/CO = 1$



1,2,3,4,5,6 denote order in which experiment was performed

Fig. 20. Effect of CO_2 Pressure on Reaction Rate



Numbers on plot denote order in which experiment was performed

Fig. 21 CH_3CHO TPSR

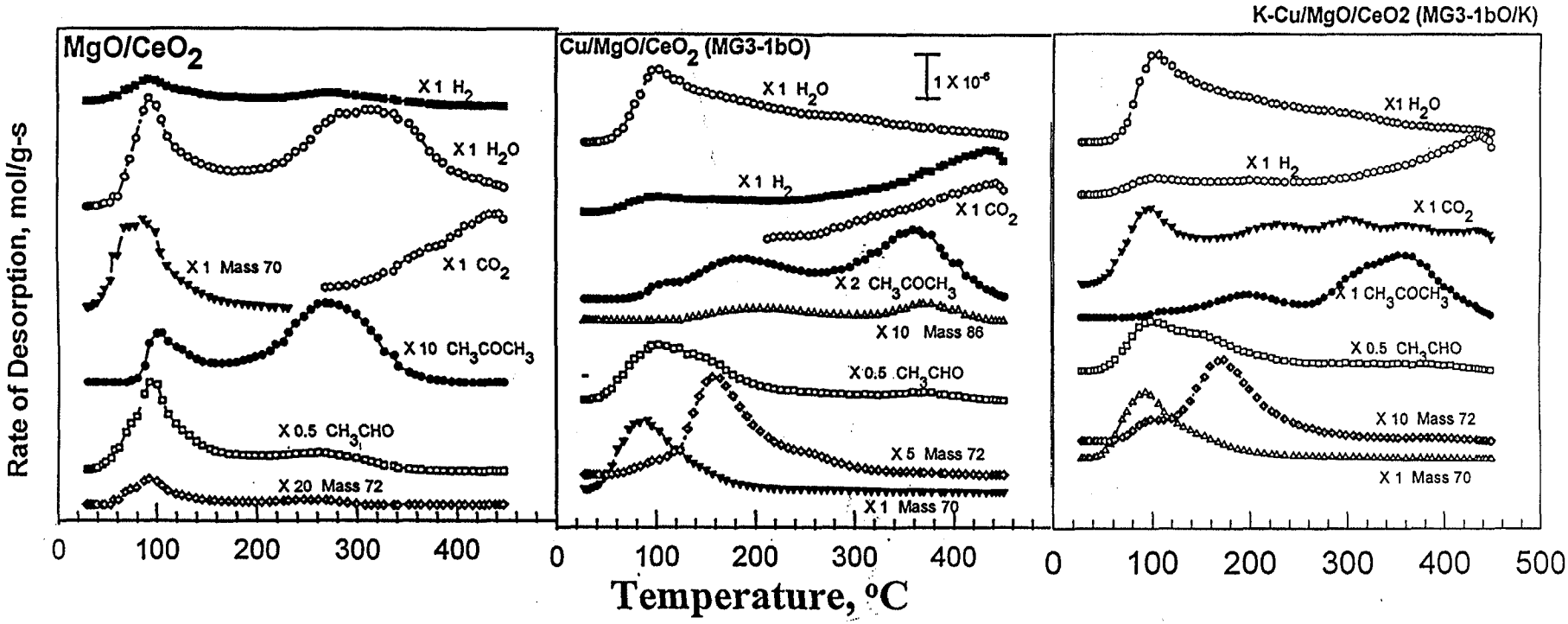


Fig. 22 Acetaldehyde TPSR on K-Cu/MgO/CeO_2

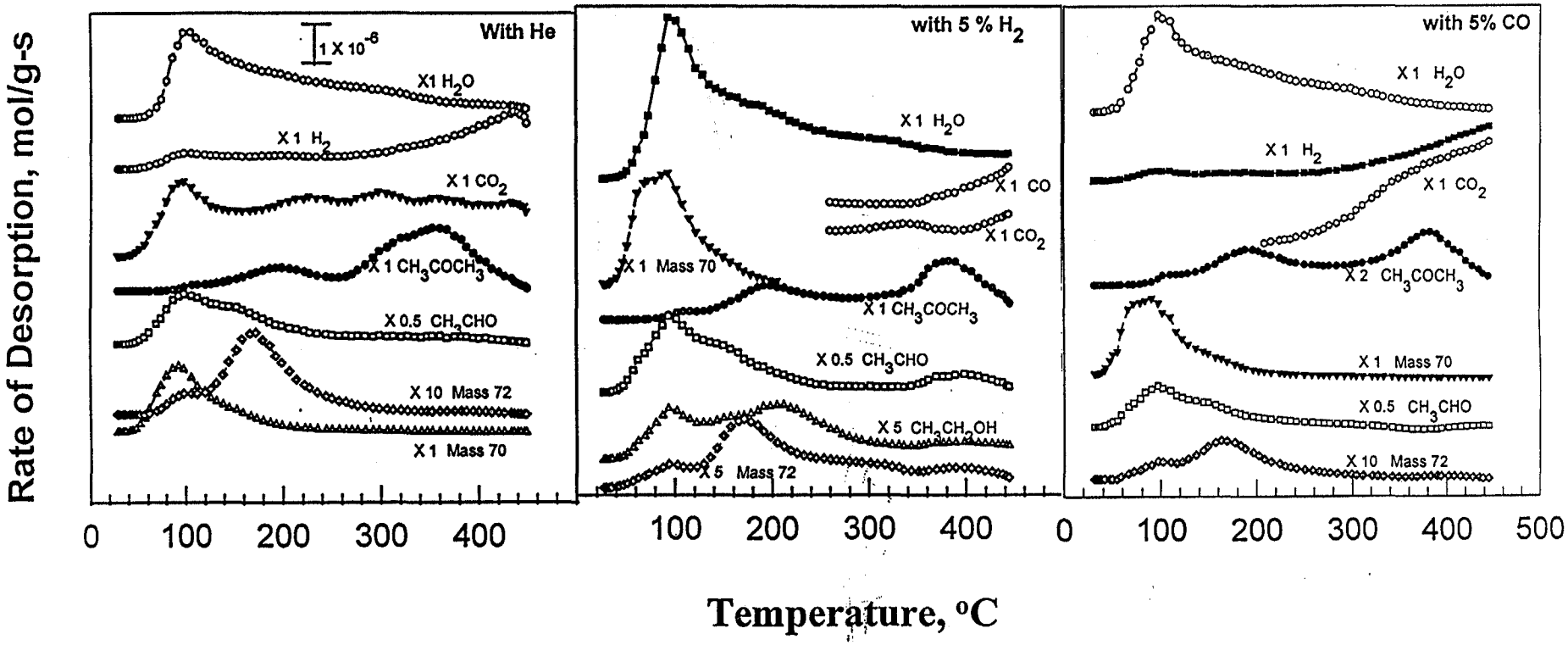


Fig.24 Ethanol TPSR

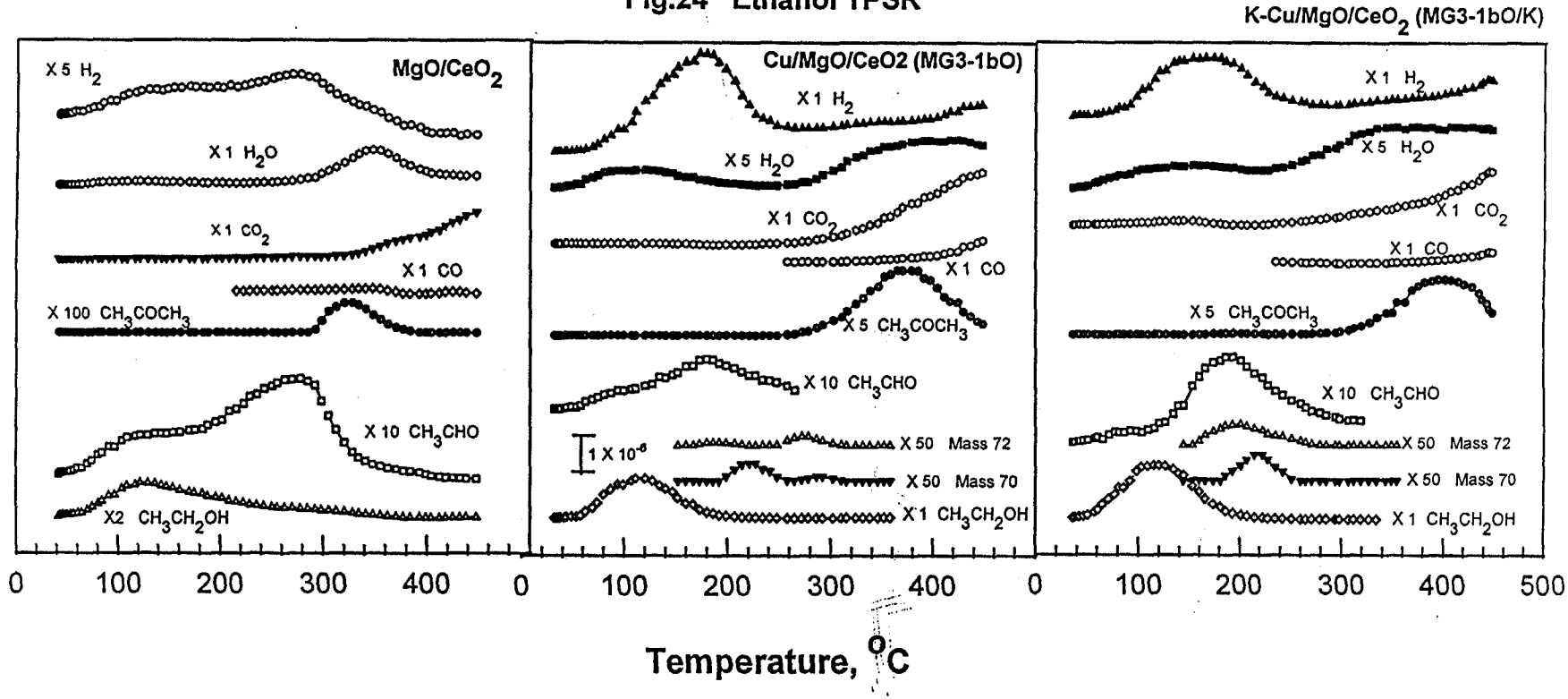


Fig. 25 Ethanol TPSR over Cu/MgO (MG3-5 O)

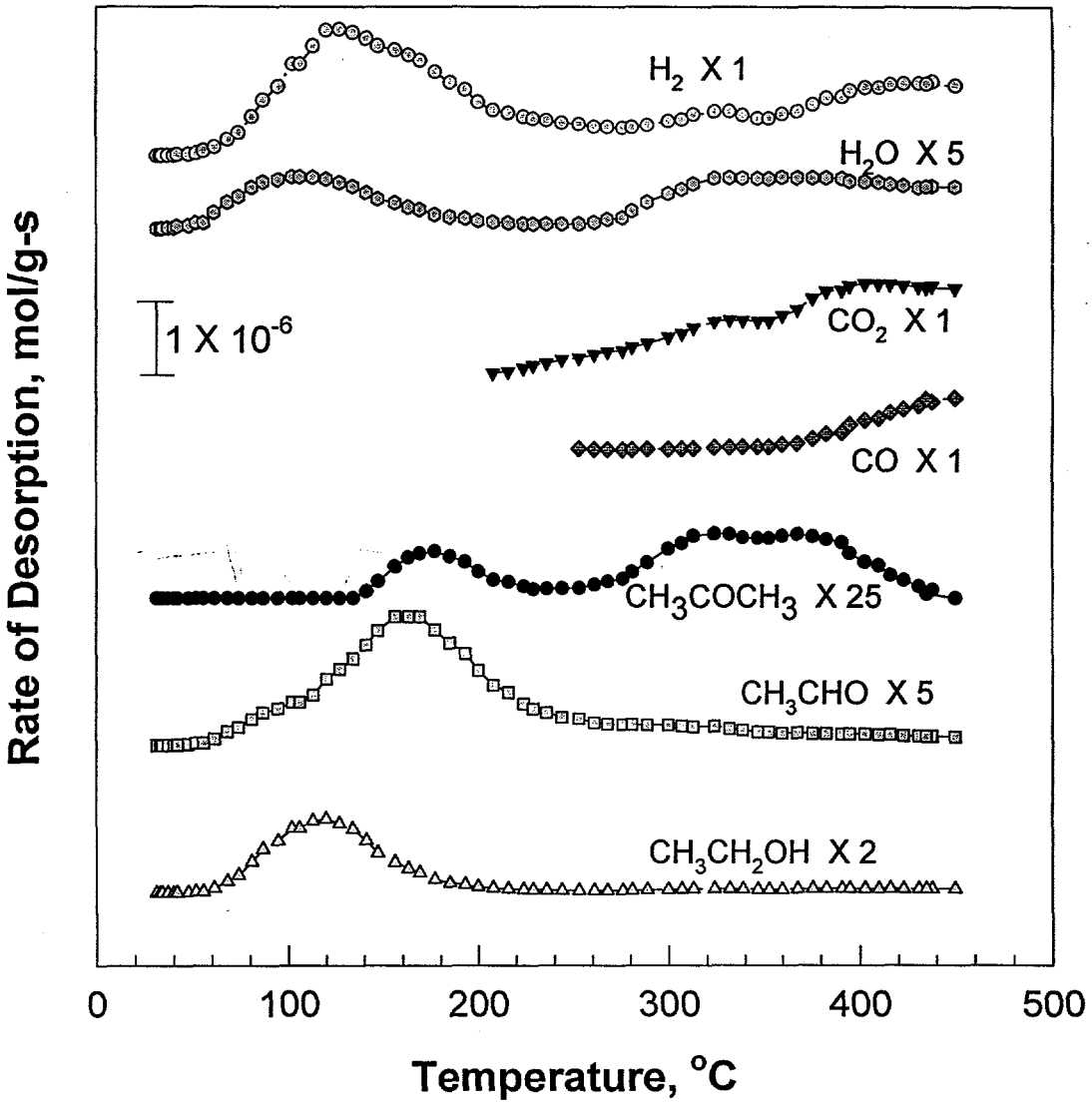


Fig.26 Ethanol TPSR over K-Cu/MgO/CeO_2 (MG3-1bO/K)

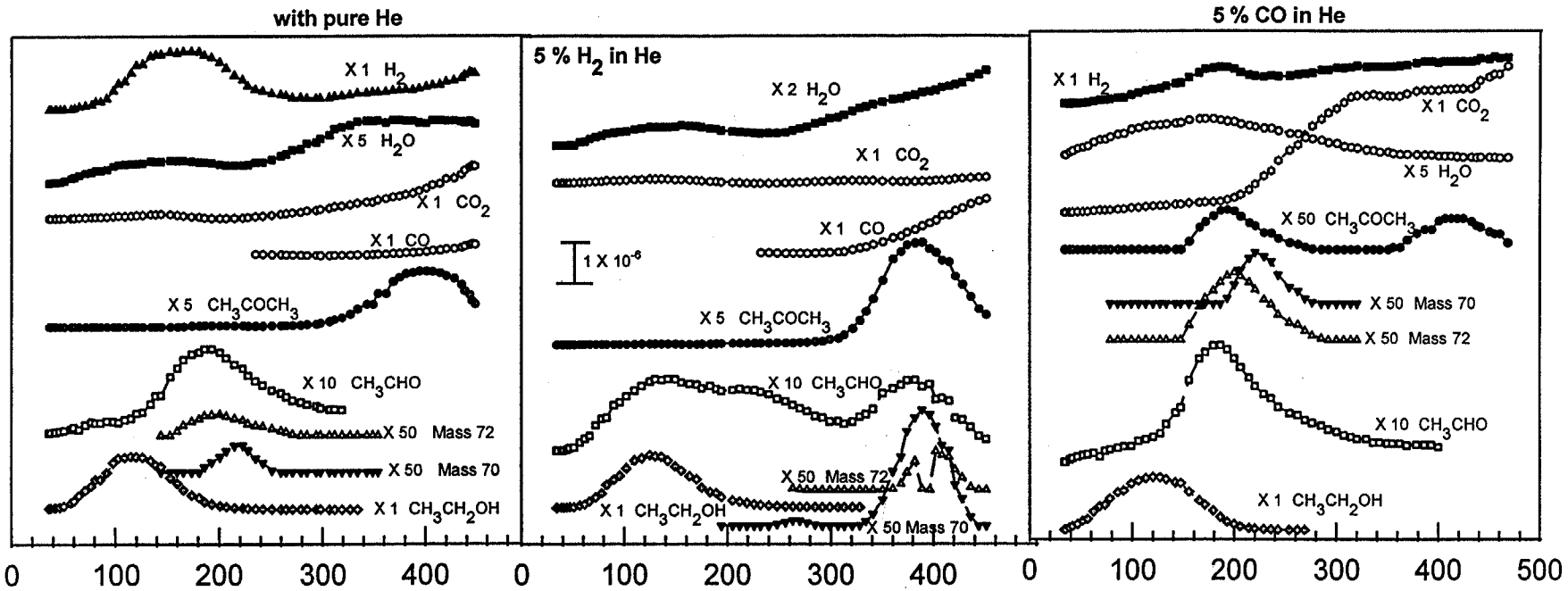
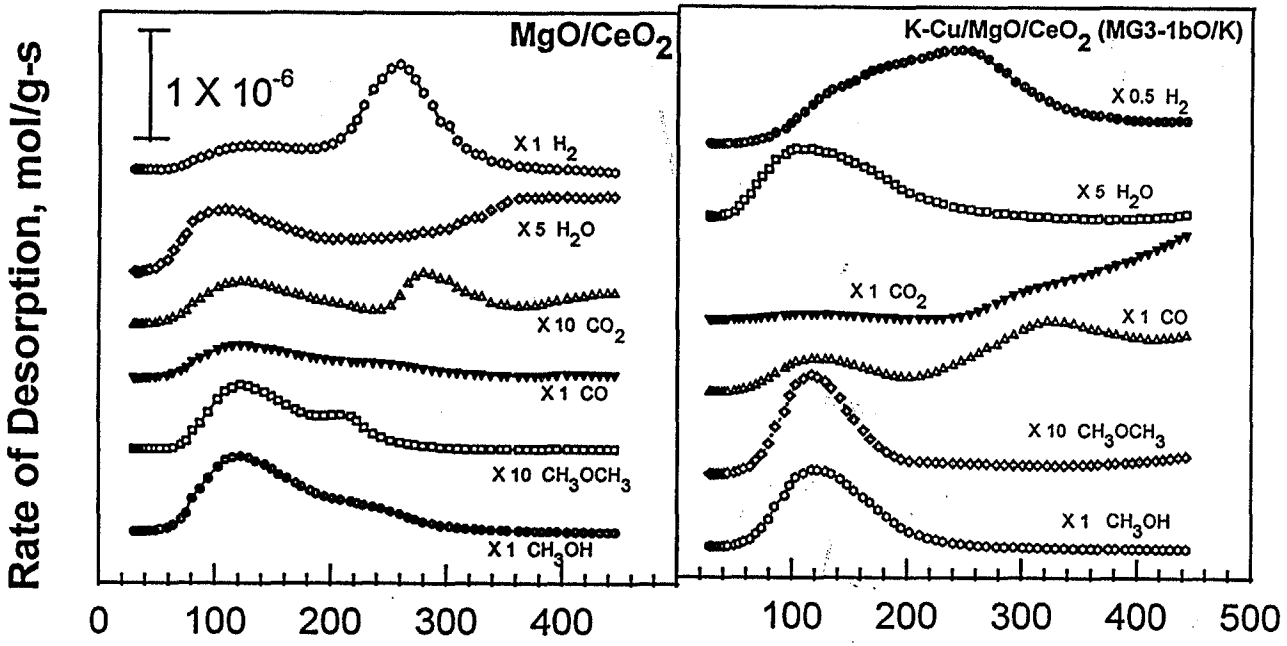


Fig. 27 CH_3OH TPSR



1. TITLE ISOBUTANOL- METHANOL MIXTURE FROM SYNGAS	2. REPORTING PERIOD Jan. 1, 1996 to Mar. 31, 1996	3. IDENTIFICATION NUMBER DE-AC22-PC94PC066
2. PARTICIPANT NAME AND ADDRESS Department of Chemical Engineering University of California- Berkeley, Berkeley, CA 94720	5. COST PLAN DATE Apr. 12, 1996	6. START DATE OCT 1994 7. COMPLETION DATE OCT 1997

8. Element code	9. Reporting element	ACCRUED COSTS				ESTIMATED ACCRUED COSTS							12. Total contract Value	13. Variance
		Reporting period		Cumulative to date		a.total this fiscal year	b. balance of fiscal year	c. FY96 (1)	d. FY 97 (2)	(3)		e. total		
		a. Actual	b. Plan	c. Actual	d. Plan									
	1. Total (Direct material)	18,949	22,777	59,853	119,597	35,060	56,049	91,109	94,782			210,684	259,929	49,245
	a) Purchased Parts	12,217	9,106	51,826	39,763	28,257	8,168	36,425	40,200			100,194	98,175	-2,019
	b) Subcontracted Items	2,114	13,670	2,114	79,833	2,114	52,565	54,679	54,582			109,261	161,754	52,493
	c) Other	4,618	0	5,913	0	4,689	0	0	0			5,913	0	-5,913
	2. Material Overhead	0	0	0	0	0	0	0	0			0	0	0
	3. Direct Labor 'Total	15,635	20,892	76,261	122,136	29,640	53,929	83,569	92,812			223,002	256,725	33,723
	4. Labor Overhead	0	0	0	0	0	0	0	0			0	0	0
	5. Fringe Benefits	1,828	3,350	8,966	19,468	3,641	9,759	13,400	15,368			34,093	41,538	7,445
	6. Special Testing	388	0	433	0	433	0	0	0			433	0	-433
	7. Special Equipment	15,402	2,000	285,980	256,000	41,802	-33,802	8,000	0			252,178	260,000	7,822
	8. Travel	2,426	1,629	5,882	9,463	3,694	2,821	6,515	7,020			15,723	19,740	4,017
	9. Consultants	0	0	0	0	0	0	0	0			0	0	0
	10. Other Direct costs	0	6,114	0	35,518	0	24,455	24,455	25,677			50,132	73,422	23,290
	11. Direct costs and Overhead	54,627	56,761	438,941	562,180	114,270	112,774	227,044	235,653			787,368	911,354	123,986
	12. General and Administrative Expense '49.5 %	19,573	20,505	76,215	124,747	36,162	45,858	82,020	90,358			212,430	256,108	43,678
	13. Facilities Capital Cost of Money	0	0	0	0	0	0	0	0			0	0	0
	14. Total Estimated Cost	74,200	77,266	515,157	686,926	150,432	158,630	309,062	326,008			999,795	1,167,462	167,667
	15. Fee	0	0	0	0	0	0	0	0			0	0	0
	16. Cost Sharing	9,786	9,949	204,163	232,953	15,408	24,389	39,797	56,789			285,341	301,651	16,310
	17. Total estimated DOE funds spent = Item 14-Item 16	64,414	67,316	310,994	453,974	135,024	134,241	269,265	269,219			714,454	865,811	151,357
14. Total		64,414	67,316	310,994	453,974	135,024	134,241	269,265	269,219			714,454	865,811	151,357

15. DOLLARS EXPRESSED IN	16. SIGNATURE OF PARTICIPANT PROJECT MANAGER AND DATE	17. SIGNATURE OF PARTICIPANT'S AUTHORIZED FINANCIAL SERVICE REPRESENTATIVE AND DATE
One U.S. Dollar		Lourdes J. Ferrer 4/12/96

DOE F 1332.3
(11-84)

U.S. DEPARTMENT OF ENERGY
MILESTONE SCHEDULE ☐ PLAN ☒ REPORT

FORM APPROVED
OMB 1901-1400

1. TITLE	2. REPORTING PERIOD	3. IDENTIFICATION NUMBER
ISOBUTANOL METHANOL MIXTURE FROM SYNGAS	Jan 1, 1996 - March 31, 1996	DE - AC22 - PC94PC066

4. PARTICIPANT NAME AND ADDRESS	5. START DATE	6. COMPLETION DATE
Department of Chemical Engineering University of California - Berkeley	Oct 1994	Sept 1997

7. ELEMENT CODE	8. REPORTING ELEMENT	9. DURATION	10. PERCENT COMPLETE a Plan	b Actual
		94 — 95 — 96 — 97 O N D Q2 Q3 Q4 O N D J F M A M J J A S Q1 Q2 Q3 Q4		
	Task 3	Complete design, construction and start-up of packed bed reactor module	100	100
	Task 2	Prepare Cu-based catalyst compositions and characterize structure, surface area, and effectiveness of several synthetic approaches	100	100
	Task 2	Choose four promising materials for catalyst evaluation	100	100
	Task 3	Construct recirculating reactor module Establish reaction pathways and rate-determining steps	100	100
	Tasks 2 & 3	Identify catalyst components necessary to catalyze rate-determing steps that have been determined	100	80
	Tasks 2 & 3	Identify synthetic techniques to increase the reactivity and accessibility of such required sites	100	80
	Task 4	Complete construction and start-up of temperature programmed surface reaction apparatus and design of high-pressure infrared cell	100	100
	Task 4	Design and construction of high-pressure infrared cell	100	70
	Task 4	Calibrate between UCB and APCI laboratories by testing two selected catalysts in slurry reactors	100	20
	Task 2	Determine the density and reactivity of the required sites and implement synthetic methods to improve them	25	25

DOE F 1332.3
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		94: O N D Q2 Q3 Q4 · 95: O N D J F M A M J J A S Q1 Q2 Q3 Q4 · 96: Q1 Q2 Q3 Q4 · 97:		
	Task 4	Identify reaction intermediates by TPSR and high pressure infrared methods	20	20
	Tasks 3 & 5	Identify catalysts with highest isoalcohol yields (two) and evaluate at conditions resembling envisioned commercial practice.	20	15
	Task 5	Assess economic viability of these catalytic materials	0	0
	Task 5	Complete testing of at least two selected catalysts in slurry reactors.	0	0
	Tasks 3 & 5	Choose two materials for detailed studies of the reaction mechanism and of optimum synthetic protocols	0	0
	Tasks 3 & 5	Complete mechanistic studies on most promising materials	0	0
	Tasks 2 & 5	Develop synthetic procedures that can be carried out on a commercial scale Suggest a range of catalyst compositions for future study.	0	0
	Task 5	Complete testing of the two selected catalytic materials	0	0
	Task 5	Assess future research requirements, technical readiness and economic viability of the most promising approach	0	0
		Produce final report	0	0