Electronic Supplementary Material (ESI) for Catalysis Science & Technology
This journal is © The Royal Society of Chemistry 2013

Journal Name

Dynamic Article Links ▶

Cite this: DOI: 10.1039/c0xx00000x

www.rsc.org/xxxxxx

ARTICLE TYPE

Electronic Supplementary Information

Impact of K and Ba promoters on CO_2 hydrogenation over Cu/Al_2O_3 catalysts at high pressure

Atul Bansode,[a] Bruno Tidona,[b] Philipp Rudolf von Rohr,[b] and Atsushi Urakawa[a,*]

[a] *Institute of Chemical Research of Catalonia (ICIQ), Av. Països Catalans 16, 43007 Tarragona, Spain*
[b] *Institute of Process Engineering, ETH Zurich, CH-8092 Zurich, Switzerland*
** Corresponding author: Fax: +34 977 920 224, E-mail address: aurakawa@iciq.es*

Contents

Table S1. CO_2 conversion, selectivity, and yield for Cu/Al_2O_3 catalyst under different conditions of temperature and pressure at GHSV = 4000 h^{-1}, H_2/CO_2 = 3.8/1**.**

Temp. / K	Pressure / MPa	Conversion / %	Selectivity / %				Yield / mg· g_{cat}^{-1}· h^{-1}			
			CO	$HCOOCH_3$	CH_3OH	CH_3OCH_3	CO	$HCOOCH_3$	CH_3OH	CH_3OCH_3
443	0.4	0.5*	87.9	-	11.2	0.9	12.6	-	1.8	0.2
473	0.4	0.7*	64.7	-	14.8	20.5	12.7	-	3.3	6.6
503	0.4	2.2	73.9	-	10.5	15.6	43.2	-	7.0	15.0
533	0.4	4.0	86.1	-	6.0	7.9	92.2	-	7.4	13.9
553	0.4	7.6	92.0	-	3.9	4.0	185.8	-	9.0	13.3
443	3	0.7*	35.5	0.8	60.3	3.3	6.8	0.3	13.2	1.0
473	3	1.2	46.7	0.2	42.6	10.5	14.2	0.1	14.9	5.3
503	3	4.0	62.2	0.0	18.8	18.9	65.4	0.1	22.6	32.8
533	3	11.3	79.3	-	6.0	14.7	238.1	-	20.5	72.6
553	3	21.3	86.2	-	3.6	10.2	486.0	-	23.1	94.9
443	10	0.8*	15.9	2.1	80.0	2.1	3.4	1.0	19.5	0.7
473	10	2.4	45.3	0.7	46.2	7.8	29.9	0.9	33.7	8.2
503	10	12.1	76.6	0.1	11.9	11.4	245.7	0.8	43.5	60.1
533	10	16.3	85.2	-	4.5	10.3	368.5	-	22.2	73.2
553	10	22.4	83.6	-	3.0	13.4	495.2	-	20.1	130.9
443	36	3.6	26.9	3.1	69.5	0.5	25.3	6.2	75.0	0.8
473	36	8.4	60.1	2.0	37.3	0.6	121.5	8.6	103.4	2.0
503	36	13.1	85.6	0.2	13.4	0.7	297.9	1.8	53.4	4.2
533	36	20.3	92.7	0.1	5.7	1.6	497.5	0.6	35.2	13.8
553	36	29.6	91.7	0.0	4.5	3.8	718.2	0.6	39.9	48.7

"-" signifies that no product was observed. The condition, where "*" is placed in CO_2 conversion, denotes that product concentration and/or CO_2 conversion are close to the detection limit

Journal Name

Dynamic Article Links ▶

Cite this: DOI: 10.1039/c0xx00000x

www.rsc.org/xxxxxx

ARTICLE TYPE

Table S2. CO_2 conversion, selectivity, and yield for Cu-K/Al_2O_3 catalyst under different conditions of temperature and pressure at GHSV = 4000 h^{-1}, H_2/CO_2 = 3.8/1.

Temp. / K	Pressure / MPa	Conversion / %	Selectivity / %				Yield / mg· g_{cat}^{-1}· h^{-1}			
			CO	$HCOOCH_3$	CH_3OH	CH_3OCH_3	CO	$HCOOCH_3$	CH_3OH	CH_3OCH_3
443	0.4	0.4*	70.2	-	29.8	-	7.9	-	3.9	-
473	0.4	1.4	84.7	-	15.3	-	32.1	-	6.6	-
503	0.4	2.6	95.3	-	4.7	-	64.9	-	3.7	-
533	0.4	5.0	98.8	-	1.2	-	129.5	-	1.8	-
553	0.4	10.7	99.0	-	1.0	-	280.6	-	3.1	-
443	3	0.9*	75.2	-	24.8	-	17.5	-	6.6	-
473	3	2.2	89.2	-	10.8	-	52.2	-	7.3	-
503	3	4.2	97.4	-	2.6	-	107.3	-	3.3	-
533	3	10.3	98.1	-	1.9	-	268.5	-	5.8	-
553	3	13.7	99.0	-	1.0	-	357.9	-	4.3	-
443	10	1.7	94.8	-	5.2	-	42.0	-	2.7	-
473	10	3.6	95.8	-	4.2	-	91.3	-	4.6	-
503	10	7.4	97.2	-	2.8	-	191.1	-	6.3	-
533	10	14.1	99.0	-	1.0	-	367.9	-	4.4	-
553	10	20.7	99.1	-	0.9	-	543.0	-	5.5	-
443	36	2.2	91.7	-	8.3	-	52.2	-	5.4	-
473	36	8.9	95.9	-	4.1	-	225.5	-	11.0	-
503	36	14.9	98.5	-	1.5	-	387.5	-	6.9	-
533	36	22.8	98.5	-	1.5	-	595.0	-	10.6	-
553	36	28.6	97.9	-	2.1	-	739.6	-	18.2	-

"-" signifies that no product was observed. The condition, where "*" is placed in CO_2 conversion, denotes that product concentration and/or CO_2 conversion are close to the detection limit

This journal is © The Royal Society of Chemistry 2013
Journal Name
Dynamic Article Links ►

Cite this: DOI: 10.1039/c0xx00000x

www.rsc.org/xxxxxx

ARTICLE TYPE

Table 3 CO_2 conversion, selectivity, and yield for Cu-Ba/Al_2O_3 catalyst under different conditions of temperature and pressure at GHSV = 4000 h^{-1}, H_2/CO_2 = 3.8/1**.**

Temp. / K	Pressure / MPa	Conversion / %	Selectivity / %				Yield / mg· g_{cat}^{-1}· h^{-1}			
			CO	$HCOOCH_3$	CH_3OH	CH_3OCH_3	CO	$HCOOCH_3$	CH_3OH	CH_3OCH_3
443	0.4	0.1*	72.5	-	27.8	0.0	2.3	-	1.0	0.0
473	0.4	1.3	70.3	-	29.3	0.4	24.6	-	11.8	0.2
503	0.4	2.7	88.6	-	11.2	0.1	64.4	-	9.4	0.2
533	0.4	9.3	95.5	-	4.4	0.0	234.7	-	12.6	0.2
553	0.4	16.2	98.1	-	1.9	0.0	419.9	-	9.3	0.1
443	3	0.4*	22.4	0.5	77.1	0.0	2.5	0.1	9.8	0.0
473	3	1.6	36.4	0.4	62.8	0.0	15.2	0.3	30.0	0.3
503	3	4.7	69.6	0.1	29.7	0.0	87.1	0.2	42.5	1.2
533	3	11.8	89.6	0.0	10.0	0.0	279.7	0.1	35.5	2.0
553	3	18.2	93.4	-	6.4	0.0	449.0	0.0	35.0	1.9
443	10	0.6*	26.0	2.1	71.9	0.0	4.3	0.7	13.7	0.0
473	10	2.8	36.8	0.7	62.2	0.4	26.8	1.0	51.9	0.5
503	10	7.4	80.2	0.2	19.0	0.6	156.2	0.7	42.4	2.0
533	10	17.1	92.9	0.1	6.5	0.5	420.2	0.5	33.5	4.0
553	10	25.2	89.6	0.1	9.3	1.0	598.1	1.1	70.7	11.4
443	36	1.7	17.4	10.3	72.3	0.0	7.8	9.9	37.1	0.0
473	36	4.3	38.3	4.3	57.2	0.1	43.4	10.5	74.1	0.2
503	36	12.4	84.0	0.9	15.1	0.2	274.0	6.0	56.5	1.0
533	36	22.9	93.8	0.1	5.8	0.2	567.6	1.6	40.2	2.4
553	36	33.7	95.4	0.1	4.1	0.4	850.8	1.5	41.9	5.7

"-" signifies that no product was observed. The condition, where "*" is placed in CO_2 conversion, denotes that product concentration and/or CO_2 conversion are close to the detection limit.