Enhancement of catalytic activity of Pd-PVP colloid for direct H_2O_2 synthesis from H_2 and O_2 in water with addition of 0.5 atom% Pt or Ir

Supporting Information

Takashi Deguchi[a], Hitoshi Yamano[b,c], Sho Takenouchi[b,d], and Masakazu Iwamoto[a,e]

[a] Research and Development Initiative, Chuo University, 1-13-27 Kasuga, Bunkyo-ku, Tokyo 112-8551, Japan.
[b] Chemical Resources Laboratory, Tokyo Institute of Technology, 4259-R1-5 Nagatsuta, Midori-ku, Yokohama 226-8503, Japan
[c] Present affiliation: Tokyo Ohka Kogyo Co., Ltd., 1590 Tabata, Samukawa-machi, Koza-gun, Kanagawa 253-0114, Japan.
[d] Present affiliation: Tanaka Kikinzoku Kogyo K.K., 2-14 Nagatoro, Hiratsuka, Kanagawa 254-0021, Japan.
[e] Present affiliation: Research Institute for Science and Engineering, Waseda University, 3-4-1 Okubo, Shinjuku-ku, Tokyo 169-8555, Japan.

S1. Experimental Details

All the data sheets describing the experimental details of the H_2-O_2 reaction are shown in the following pages. The items contained in the data sheets are:

1) Concentrations of the catalysts and additives charged.
2) Reaction conditions: ambient temperature (T_0), reaction temperature (T), ambient atmosphere (P_0), inner pressure (P), agitation speed.
3) Feed rates of H_2, O_2 and N_2 (set and calibrated). "Feed gas measurement" describes the calibration data obtained by measuring the flow rate of each gas using a soap-film flow meter before the reaction.
4) Results of GC calibration. The combined feed gas was put in GC three times before and after the reaction run respectively, and the ratios of sensitivity of H_2 and O_2 against N_2 were determined as the averages.
5) GC counts of H_2, O_2 and N_2 at every sampling time.
6) Corrected elapsed time, $t_{correct}$, and reaction parameters at every sampling time: outlet flows, conversions, partial pressures, reaction rates all of H_2 and O_2, as well as $d[H_2O_2]/dt$, $\Sigma[H_2]$ (= $\int r_{H2} dt$), $[H_2O_2]$, S_e, $\Sigma_1/[H_2O_2]$ and $\Sigma_2/[H_2O_2]$.
7) Values of S_f and k_d[Cat] calculated from $\Sigma_1/[H_2O_2]$ and $\Sigma_2/[H_2O_2]$ as well as the value of R^2.

H_2O_2 Synthesis Data Sheet

Entry No. 1 (Exp. Y01) Employed in: Table. 1 Table 2 Fig. 3 Fig. 4 Fig. 5 Fig. 9 Fig. 10 Fig. 11

Catalyst, Additives			Reaction conditions		Gas feed rate (sccm)				
Name	Conc.	(Unit)	T_0 (℃)	22.0		H_2	O_2	N_2	Sum
Pd-PVP	8.33	(mg/L)	T (℃)	29.9	Set	10.00	20.00	20.00	50.00
			P_0 (hPa)	1005.2	Calibrated	10.20	18.55	19.86	
H_2SO_4	0.01	(N)	P (hPa)	1012.5	Determination of final $[H_2O_2]$		Sample (g)	Absorbance (—)	$[H_2O_2]$ (mmol L^{-1})
NaBr	0.001	(N)	Agitation (rpm)	1200					
							0.958	0.774	27.73
Comment: Catalyst activation: H_2 gas 20 sccm at 303 K for 40 min.					Analysis of H_2O_2 formation selectivity and H_2O_2 destruction rate			S_f (—)	0.8579
								k_d[Cat] (h^{-1})	0.5291
								R^2	0.9995

GC calibration		GC count			Ratio of sensitivity (toward N_2)				Feed gas measurement	
Timing	No.	H_2	O_2	N_2	H_2		O_2			
Before reaction	1	964827	194744	171252	0.0911	0.0911	0.821	0.823	T_a (℃)	22.6
	2	965037	194687	171494	0.0912		0.823		P_0 (hPa)	1005.0
	3	965480	194643	171485	0.0912		0.823		Flow	(cc/min)
After reaction	4	964401	193957	171086	0.0911		0.824		H_2	11.44
	5	964392	194047	171179	0.0911		0.824		O_2	20.81
	6	964705	194069	171063	0.0910		0.823		N_2	22.28

Time				GC count			$t_{correct.}$	Outlet flow (sccm)		Conversion(%)	
H	M	S	min.	H_2	O_2	N_2	(min)	H_2	O_2	H_2	O_2
11	1	32	4.0	490681	110798	269198	0.00	7.75	16.29	24.02	12.19
11	11	34	14.0	762344	177997	191470	9.26	7.69	16.30	24.59	12.10
11	21	38	24.1	776020	183873	185204	19.32	7.62	16.32	25.22	12.00
11	31	40	34.1	771608	184708	184809	29.36	7.56	16.33	25.89	11.93
11	41	44	44.2	766413	185093	184795	39.42	7.51	16.37	26.38	11.74
11	51	46	54.2	759836	185414	185099	49.46	7.43	16.37	27.13	11.73
12	1	50	64.3	752909	185650	185350	59.52	7.35	16.37	27.90	11.74
12	11	52	74.3	745289	185930	186025	69.56	7.25	16.33	28.88	11.93
12	21	56	84.4	738716	186166	185873	79.62	7.19	16.37	29.45	11.75
12	31	58	94.4	733217	186481	186299	89.66	7.12	16.36	30.14	11.80
12	42	2	104.5	727299	186869	186772	99.72	7.05	16.35	30.88	11.84
12	52	4	114.5	722224	187136	187009	109.76	6.99	16.35	31.45	11.82
13	2	8	124.6	717363	187425	187236	119.82	6.93	16.36	31.99	11.80

$t_{correct.}$	Partial pressure (kPa)		Rate (mmol L^{-1} h^{-1})		$d[H_2O_2]/dt$	$\Sigma[H_2]$	$[H_2O_2]$	S_e	$\Sigma_2/[H_2O_2]$	$\Sigma_1/[H_2O_2]$
(min)	p_{H2}	p_{O2}	r_{H2}	r_{O2}	(mmol L^{-1} h^{-1})	(mmol L^{-1})	(mmol L^{-1})	(—)	(h)	(—)
0.00	17.13	36.00	21.86	20.19	18.52	0.00	0.00		0.000	0.000
9.26	17.01	36.07	22.39	20.04	17.69	3.41	2.79	0.82	0.077	1.222
19.32	16.89	36.15	22.96	19.87	16.79	7.22	5.68	0.79	0.163	1.270
29.36	16.76	36.23	23.57	19.76	15.95	11.11	8.42	0.76	0.250	1.319
39.42	16.65	36.32	24.02	19.45	14.87	15.10	11.01	0.73	0.339	1.372
49.46	16.51	36.38	24.70	19.43	14.16	19.17	13.44	0.70	0.430	1.427
59.52	16.37	36.44	25.40	19.44	13.49	23.38	15.76	0.67	0.522	1.484
69.56	16.19	36.48	26.30	19.75	13.21	27.70	17.99	0.65	0.614	1.540
79.62	16.07	36.57	26.81	19.45	12.09	32.15	20.11	0.63	0.708	1.599
89.66	15.95	36.62	27.44	19.54	11.64	36.69	22.10	0.60	0.804	1.660
99.72	15.81	36.67	28.11	19.60	11.10	41.35	24.00	0.58	0.902	1.723
109.76	15.70	36.72	28.63	19.58	10.53	46.09	25.81	0.56	1.000	1.786
119.82	15.59	36.78	29.12	19.53	9.94	50.94	27.53	0.54	1.100	1.850

H_2O_2 Synthesis Data Sheet

Entry No. 2 (Exp. Y146) Employed in: Table. 1

Catalyst, Additives			Reaction conditions		Gas feed rate (sccm)				
Name	Conc.	(Unit)	T_0 (℃)	23.4		H_2	O_2	N_2	Sum
Pd-PVP	8.33	(mg/L)	T (℃)	29.9	Set	10.00	20.00	20.00	50.00
$RuCl_3$	0.0883	(mg-Ru/L)	P_0 (hPa)	1009.0	Calibrated	10.12	18.55	19.86	48.53
H_2SO_4	0.01	(N)	P (hPa)	1016.3	Determination of final $[H_2O_2]$		Sample (g)	Absorbance (—)	$[H_2O_2]$ (mmol L^{-1})
NaBr	0.001	(N)	Agitation (rpm)	1201					
							0.680	0.499	24.77
Comment: Catalyst activation: H_2 gas 20 sccm at 303 K for 40 min.					Analysis of H_2O_2 formation selectivity and H_2O_2 destruction rate			S_f (—)	0.7622
								k_d[Cat] (h^{-1})	0.5778
								R^2	1.0000

GC calibration		GC count			Ratio of sensitivity (toward N_2)				Feed gas measurement	
Timing	No.	H_2	O_2	N_2	H_2		O_2			
Before reaction	1	993585	199939	172952	0.0887	0.0883	0.808	0.808	T_a (℃)	23.4
	2	992977	199871	172998	0.0888		0.808		P_0 (hPa)	1008.2
	3	993084	199849	172923	0.0887		0.808		Flow	(cc/min)
After reaction	4	994104	199826	172955	0.0886		0.808		H_2	11.36
	5	993947	199885	173029	0.0887		0.809		O_2	20.83
	6	1014427	198796	172016	0.0864		0.808		N_2	22.30

Time				GC count			$t_{correct.}$	Outlet flow (sccm)		Conversion(%)	
H	M	S	min.	H_2	O_2	N_2	(min)	H_2	O_2	H_2	O_2
15	39	8	4.0	545593	118963	268077	0.00	7.83	16.54	22.57	10.82
15	49	12	14.1	796646	185604	191542	9.53	7.73	16.52	23.61	10.93
15	59	14	24.1	805918	190683	186420	19.57	7.62	16.50	24.71	11.04
16	9	18	34.2	798774	191534	186595	29.63	7.51	16.48	25.80	11.17
16	19	20	44.2	788417	191683	186917	39.67	7.40	16.46	26.88	11.26
16	29	24	54.3	779440	192004	187538	49.73	7.29	16.44	27.96	11.40
16	39	26	64.3	770892	192271	188090	59.77	7.19	16.41	28.96	11.54
16	49	30	74.4	761810	192413	188490	69.83	7.09	16.39	29.94	11.66
16	59	32	84.4	754472	192770	189037	79.87	7.00	16.37	30.82	11.75
17	9	36	94.5	746987	192967	189353	89.93	6.92	16.36	31.62	11.81
17	19	38	104.5	740593	193159	189625	99.97	6.85	16.35	32.30	11.85
17	29	42	114.6	735205	193524	190030	110.03	6.78	16.35	32.94	11.87
17	39	44	124.6	730828	193647	190120	120.07	6.74	16.35	33.37	11.86

$t_{correct.}$	Partial pressure (kPa)		Rate (mmol L^{-1} h^{-1})		$d[H_2O_2]/dt$	$\Sigma[H_2]$	$[H_2O_2]$	S_e	$\Sigma_2/[H_2O_2]$	$\Sigma_1/[H_2O_2]$
(min)	p_{H2}	p_{O2}	r_{H2}	r_{O2}	(mmol L^{-1} h^{-1})	(mmol L^{-1})	(mmol L^{-1})	(—)	(h)	(—)
0.00	17.25	36.43	20.38	17.92	15.45	0.00	0.00		0.000	0.000
9.53	17.07	36.49	21.33	18.10	14.87	3.31	2.41	0.73	0.079	1.376
19.57	16.87	36.55	22.32	18.29	14.27	6.96	4.85	0.70	0.165	1.437
29.63	16.68	36.61	23.30	18.50	13.70	10.79	7.19	0.67	0.251	1.500
39.67	16.48	36.68	24.28	18.64	13.00	14.77	9.42	0.64	0.339	1.567
49.73	16.29	36.73	25.25	18.88	12.51	18.92	11.56	0.61	0.429	1.636
59.77	16.11	36.78	26.15	19.11	12.07	23.22	13.62	0.59	0.519	1.705
69.83	15.93	36.83	27.05	19.31	11.58	27.69	15.60	0.56	0.610	1.774
79.87	15.77	36.88	27.84	19.47	11.10	32.27	17.50	0.54	0.702	1.844
89.93	15.62	36.94	28.56	19.56	10.56	37.00	19.32	0.52	0.796	1.916
99.97	15.49	36.98	29.18	19.62	10.07	41.83	21.04	0.50	0.891	1.988
110.03	15.37	37.03	29.75	19.66	9.57	46.78	22.69	0.49	0.988	2.062
120.07	15.28	37.07	30.14	19.64	9.13	51.78	24.25	0.47	1.086	2.135

H_2O_2 Synthesis Data Sheet

Entry No. 3 (Exp. Y145) Employed in: Table. 1

Catalyst, Additives			Reaction conditions		Gas feed rate (sccm)				
Name	Conc.	(Unit)	T_0 (℃)	22.7		H_2	O_2	N_2	Sum
Pd-PVP	8.33	(mg/L)	T (℃)	29.9	Set	10.00	20.00	20.00	50.00
$RhCl_3$	0.04	(mg-Rh/L)	P_0 (hPa)	1008.8	Calibrated	10.12	18.55	19.86	48.53
H_2SO_4	0.01	(N)	P (hPa)	1016.1	Determination of final $[H_2O_2]$		Sample (g)	Absorbance (—)	$[H_2O_2]$ (mmol L^{-1})
NaBr	0.001	(N)	Agitation (rpm)	1202					
							0.591	0.487	27.82
Comment: Catalyst activation: H_2 gas 20 sccm at 303 K for 40 min.					Analysis of H_2O_2 formation selectivity and H_2O_2 destruction rate			S_f (—)	0.7680
								k_d[Cat] (h^{-1})	0.4663
								R^2	0.9999

GC calibration		GC count			Ratio of sensitivity (toward N_2)				Feed gas measurement	
Timing	No.	H_2	O_2	N_2	H_2		O_2			
Before reaction	1	994795	200757	173863	0.0890	0.0889	0.809	0.809	T_a (℃)	23.4
	2	994418	200311	173458	0.0889		0.809		P_0 (hPa)	1008.2
	3	991865	200349	173759	0.0892		0.810		Flow	(cc/min)
After reaction	4	995495	200356	173443	0.0888		0.809		H_2	11.36
	5	995137	200202	173151	0.0886		0.808		O_2	20.83
	6	994006	199904	172997	0.0887		0.808		N_2	22.30

Time				GC count			$t_{correct.}$	Outlet flow (sccm)		Conversion(%)	
H	M	S	min.	H_2	O_2	N_2	(min)	H_2	O_2	H_2	O_2
11	55	58	4.0	531572	118135	271544	0.00	7.31	16.07	27.78	13.35
12	6	2	14.1	768666	185329	196057	9.68	7.25	16.10	28.29	13.22
12	16	4	24.1	776263	190918	191064	19.72	7.20	16.12	28.83	13.08
12	26	8	34.2	770465	191325	190325	29.78	7.14	16.15	29.38	12.96
12	36	10	44.2	764913	191590	190226	39.82	7.10	16.18	29.86	12.79
12	46	14	54.3	759907	192189	190592	49.88	7.04	16.20	30.45	12.69
12	56	16	64.3	753159	192260	190588	59.92	6.97	16.20	31.06	12.65
13	6	18	74.3	748348	192729	190928	69.95	6.92	16.21	31.63	12.60
13	16	22	84.4	743569	192968	191067	80.02	6.87	16.22	32.11	12.55
13	26	24	94.4	739201	193301	191204	90.05	6.82	16.24	32.56	12.46
13	36	28	104.5	735128	193456	191215	100.12	6.78	16.25	32.94	12.40
13	46	30	114.5	732130	193637	191239	110.15	6.76	16.26	33.22	12.33
13	56	34	124.6	729668	194230	191570	120.22	6.72	16.29	33.56	12.21

$t_{correct.}$	Partial pressure (kPa)		Rate (mmol L^{-1} h^{-1})		$d[H_2O_2]/dt$	$\Sigma[H_2]$	$[H_2O_2]$	S_e	$\Sigma_2/[H_2O_2]$	$\Sigma_1/[H_2O_2]$
(min)	p_{H2}	p_{O2}	r_{H2}	r_{O2}	(mmol L^{-1} h^{-1})	(mmol L^{-1})	(mmol L^{-1})	(—)	(h)	(—)
0.00	16.45	36.20	25.09	22.11	19.13	0.00	0.00		0.000	0.000
9.68	16.35	36.28	25.56	21.89	18.23	4.09	3.01	0.74	0.081	1.356
19.72	16.24	36.36	26.04	21.67	17.30	8.40	5.99	0.71	0.166	1.404
29.78	16.12	36.44	26.54	21.46	16.38	12.81	8.81	0.69	0.254	1.454
39.82	16.02	36.52	26.97	21.19	15.41	17.29	11.47	0.66	0.343	1.507
49.88	15.90	36.60	27.50	21.01	14.52	21.86	13.98	0.64	0.434	1.563
59.92	15.78	36.66	28.06	20.96	13.86	26.50	16.35	0.62	0.526	1.621
69.95	15.67	36.72	28.57	20.86	13.16	31.24	18.61	0.60	0.619	1.678
80.02	15.57	36.78	29.01	20.79	12.57	36.07	20.77	0.58	0.714	1.736
90.05	15.48	36.84	29.41	20.64	11.87	40.95	22.81	0.56	0.810	1.795
100.12	15.40	36.89	29.75	20.53	11.32	45.91	24.76	0.54	0.907	1.854
110.15	15.34	36.93	30.00	20.42	10.83	50.91	26.61	0.52	1.006	1.913
120.22	15.27	36.99	30.31	20.22	10.14	55.97	28.37	0.51	1.106	1.973

H_2O_2 Synthesis Data Sheet

Entry No. 4 (Exp. Y151) Employed in: Table. 1 Fig. 3 Fig. 10 Fig. 11

Catalyst, Additives			Reaction conditions		Gas feed rate (sccm)				
Name	Conc.	(Unit)	T_0 (℃)	25.1		H_2	O_2	N_2	Sum
Pd-PVP	8.33	(mg/L)	T (℃)	30.0	Set	14.00	20.00	20.00	54.00
$IrCl_3$	0.08667	(mg-Ir/L)	P_0 (hPa)	1012.8	Calibrated	14.06	18.56	19.89	52.51
H_2SO_4	0.01	(N)	P (hPa)	1019.5	Determination of final $[H_2O_2]$		Sample (g)	Absorbance (—)	$[H_2O_2]$ (mmol L^{-1})
NaBr	0.001	(N)	Agitation (rpm)	1198					
							0.515	0.836	54.72
Comment: Catalyst activation: H_2 gas 20 sccm at 303 K for 40 min.					Analysis of H_2O_2 formation selectivity and H_2O_2 destruction rate			S_f (—)	0.5506
								k_d[Cat] (h^{-1})	0.3507
								R^2	0.9997

GC calibration		GC count			Ratio of sensitivity (toward N_2)				Feed gas measurement	
Timing	No.	H_2	O_2	N_2	H_2		O_2			
Before reaction	1	1261831	185394	160432	0.0899	0.0897	0.807	0.807	T_a (℃)	24.8
	2	1261906	185313	160326	0.0898		0.807		P_0 (hPa)	1013.0
	3	1262159	185208	160190	0.0897		0.807		Flow	(cc/min)
After reaction	4	1262024	184777	159782	0.0895		0.807		H_2	15.83
	5	1262965	184802	159882	0.0895		0.807		O_2	20.89
	6	1263508	185014	160043	0.0896		0.807		N_2	22.39

Time				GC count			$t_{correct.}$	Outlet flow (sccm)		Conversion(%)	
H	M	S	min.	H_2	O_2	N_2	(min)	H_2	O_2	H_2	O_2
16	28	56	4.0	610155	105352	273270	0.00	6.18	12.45	56.04	32.90
16	38	58	14.0	742639	159704	217092	10.87	6.15	12.55	56.24	32.35
16	49	2	24.1	732488	166040	212200	20.94	6.13	12.65	56.44	31.84
16	59	4	34.1	722380	167585	211190	30.97	6.10	12.74	56.62	31.36
17	9	8	44.2	715304	168282	210255	41.04	6.07	12.85	56.85	30.76
17	19	10	54.2	710916	168918	209720	51.07	6.05	12.93	57.01	30.32
17	29	14	64.3	711485	169869	209550	61.14	6.06	13.01	56.94	29.88
17	39	16	74.3	713281	170969	209261	71.17	6.08	13.12	56.77	29.32
17	49	20	84.4	715143	171909	208735	81.24	6.11	13.22	56.55	28.76
17	59	22	94.4	714510	171769	207316	91.27	6.15	13.30	56.29	28.33
18	9	24	104.5	719003	173303	207627	101.30	6.18	13.40	56.08	27.79
18	19	28	114.5	719836	173779	207024	111.37	6.20	13.48	55.90	27.39
18	29	30	124.6	718815	173924	206077	121.40	6.22	13.55	55.76	26.99

$t_{correct.}$	Partial pressure (kPa)		Rate (mmol L^{-1} h^{-1})		$d[H_2O_2]/dt$	$\Sigma[H_2]$	$[H_2O_2]$	S_e	$\Sigma_2/[H_2O_2]$	$\Sigma_1/[H_2O_2]$
(min)	p_{H2}	p_{O2}	r_{H2}	r_{O2}	(mmol L^{-1} h^{-1})	(mmol L^{-1})	(mmol L^{-1})	(—)	(h)	(—)
0.00	15.68	31.57	70.36	54.53	38.69	0.00	0.00		0.000	0.000
10.87	15.57	31.77	70.63	53.61	36.60	12.77	6.82	0.53	0.091	1.873
20.94	15.48	31.96	70.87	52.76	34.66	24.64	12.80	0.52	0.177	1.925
30.97	15.39	32.13	71.09	51.96	32.82	36.51	18.44	0.51	0.264	1.980
41.04	15.27	32.34	71.39	50.98	30.57	48.46	23.76	0.49	0.354	2.040
51.07	15.20	32.50	71.58	50.25	28.92	60.42	28.73	0.48	0.446	2.103
61.14	15.18	32.63	71.50	49.51	27.51	72.42	33.46	0.46	0.539	2.164
71.17	15.20	32.78	71.28	48.59	25.90	84.36	37.93	0.45	0.632	2.224
81.24	15.22	32.93	71.01	47.65	24.30	96.29	42.14	0.44	0.729	2.285
91.27	15.27	33.03	70.68	46.94	23.20	108.14	46.11	0.43	0.826	2.345
101.30	15.29	33.17	70.42	46.06	21.70	119.94	49.86	0.42	0.925	2.405
111.37	15.31	33.27	70.19	45.38	20.57	131.73	53.41	0.41	1.026	2.466
121.40	15.33	33.38	70.02	44.73	19.43	143.46	56.75	0.40	1.127	2.528

H_2O_2 Synthesis Data Sheet

Entry No. 5 (Exp. G62) Employed in: Table. 1 Fig. 3 Fig. 6 Fig. 7 Fig. 8

Catalyst, Additives			Reaction conditions		Gas feed rate (sccm)				
Name	Conc.	(Unit)	T_0 (℃)	22.2		H_2	O_2	N_2	Sum
Pd-PVP	8.33	(mg/L)	T (℃)	30.0	Set	12.50	20.00	20.00	52.50
$Pt(NH_3)_4(NO_3)_2$	0.0833	(mg-Pt/L)	P_0 (hPa)	1011.5	Calibrated	12.49	18.68	20.06	51.23
H_2SO_4	0.01	(N)	P (hPa)	1018.0	Determination of final $[H_2O_2]$		Sample (g)	Absorbance (—)	$[H_2O_2]$ (mmol L^{-1})
NaBr	0.001	(N)	Agitation (rpm)	1199					
							0.662	1.053	54.64
Comment: Catalyst activation: H_2 gas 20 sccm at 303 K for 40 min.					Analysis of H_2O_2 formation selectivity and H_2O_2 destruction rate			S_f (—)	0.7458
								k_d[Cat] (h^{-1})	0.5011
								R^2	0.9972

GC calibration		GC count			Ratio of sensitivity (toward N_2)				Feed gas measurement	
Timing	No.	H_2	O_2	N_2	H_2		O_2			
Before reaction	1	1128473	185518	161206	0.0890	0.0888	0.809	0.810	T_a (℃)	21.4
	2	1129357	185655	161357	0.0890		0.810		P_0 (hPa)	1012.8
	3	1129078	185333	161000	0.0888		0.809		Flow	(cc/min)
After reaction	4	1128936	185063	160903	0.0888		0.810		H_2	13.82
	5	1128595	184880	160584	0.0886		0.809		O_2	20.67
	6	1130586	185401	161199	0.0888		0.810		N_2	22.19

Time				GC count				$t_{correct.}$	Outlet flow (sccm)		Conversion(%)	
H	M	S	min.	H_2	O_2	N_2		(min)	H_2	O_2	H_2	O_2
12	58	8	4.0	520436	104082	270431		0.00	6.65	13.63	46.75	27.05
13	8	12	14.1	718722	162260	205753		9.84	6.56	13.68	47.51	26.76
13	18	14	24.1	720239	168236	200274		19.87	6.46	13.74	48.29	26.47
13	28	18	34.2	713149	169671	199879		29.94	6.36	13.78	49.11	26.23
13	38	20	44.2	704164	170510	199736		39.97	6.28	13.86	49.72	25.81
13	48	24	54.3	691782	171042	199936		50.04	6.16	13.89	50.65	25.65
13	58	26	64.3	675871	171563	200560		60.07	6.00	13.89	51.94	25.66
14	8	30	74.4	606121	172076	206151		70.14	5.24	13.55	58.07	27.46
14	18	32	84.4	593111	172791	207203		80.17	5.10	13.54	59.18	27.53
14	28	34	94.4	594309	173106	206749		90.20	5.12	13.59	59.00	27.24
14	38	38	104.5	597480	173393	206163		100.27	5.16	13.65	58.67	26.91
14	48	40	114.5	599495	173767	205967		110.30	5.19	13.70	58.49	26.68
14	58	44	124.6	602332	174258	205675		120.37	5.22	13.76	58.23	26.37

$t_{correct.}$	Partial pressure (kPa)		Rate (mmol L^{-1} h^{-1})		d$[H_2O_2]$/dt	$\Sigma[H_2]$	$[H_2O_2]$	S_e	$\Sigma_2/[H_2O_2]$	$\Sigma_1/[H_2O_2]$
(min)	p_{H2}	p_{O2}	r_{H2}	r_{O2}	(mmol L^{-1} h^{-1})	(mmol L^{-1})	(mmol L^{-1})	(—)	(h)	(—)
0.00	16.09	32.97	52.14	45.11	38.09	0.00	0.00		0.000	0.000
9.84	15.88	33.14	52.99	44.64	36.29	8.62	6.10	0.71	0.082	1.413
19.87	15.66	33.30	53.85	44.16	34.47	17.55	12.01	0.68	0.168	1.461
29.94	15.43	33.46	54.78	43.75	32.73	26.66	17.65	0.66	0.255	1.511
39.97	15.25	33.65	55.45	43.05	30.66	35.88	22.95	0.64	0.344	1.563
50.04	15.00	33.79	56.49	42.79	29.09	45.27	27.96	0.62	0.435	1.619
60.07	14.66	33.92	57.92	42.80	27.68	54.84	32.71	0.60	0.527	1.676
70.14	13.15	34.03	64.76	45.80	26.85	65.13	37.28	0.57	0.620	1.747
80.17	12.86	34.13	66.00	45.92	25.84	76.06	41.69	0.55	0.713	1.824
90.20	12.89	34.21	65.80	45.43	25.06	87.08	45.95	0.53	0.806	1.895
100.27	12.96	34.27	65.43	44.89	24.34	98.09	50.09	0.51	0.900	1.958
110.30	12.99	34.32	65.23	44.51	23.78	109.01	54.11	0.50	0.994	2.015
120.37	13.04	34.39	64.94	43.99	23.03	119.93	58.04	0.48	1.089	2.066

H_2O_2 Synthesis Data Sheet

Entry No. 6 (Exp. Y144) Employed in: Table. 1

Catalyst, Additives			Reaction conditions		Gas feed rate (sccm)				
Name	Conc.	(Unit)	T_0 (℃)	22.0		H_2	O_2	N_2	Sum
Pd-PVP	8.33	(mg/L)	T (℃)	29.9	Set	10.00	20.00	20.00	50.00
$HAuCl_4$	0.0857	(mg-Au/L)	P_0 (hPa)	1012.6	Calibrated	9.94	18.61	19.89	48.44
H_2SO_4	0.01	(N)	P (hPa)	1020.0	Determination of final $[H_2O_2]$		Sample (g)	Absorbance (—)	$[H_2O_2]$ (mmol L^{-1})
NaBr	0.001	(N)	Agitation (rpm)	1200					
							0.969	0.730	25.41
Comment: Catalyst activation: H_2 gas 20 sccm at 303 K for 40 min.					Analysis of H_2O_2 formation selectivity and H_2O_2 destruction rate			S_f (—)	0.8846
								k_d[Cat] (h^{-1})	0.4068
								R^2	0.9997

GC calibration		GC count			Ratio of sensitivity (toward N_2)				Feed gas measurement	
Timing	No.	H_2	O_2	N_2	H_2		O_2			
Before reaction	1	999707	201760	174721	0.0873	0.0872	0.810	0.810	T_a (℃)	22.7
	2	999076	201122	174141	0.0871		0.810		P_0 (hPa)	1013.6
	3	997755	200981	174021	0.0872		0.810		Flow	(cc/min)
After reaction	4	993864	200031	173245	0.0871		0.811		H_2	11.06
	5	994427	200152	173276	0.0871		0.810		O_2	20.71
	6	993444	200037	173269	0.0872		0.811		N_2	22.13

Time				GC count			$t_{correct.}$	Outlet flow (sccm)		Conversion(%)	
H	M	S	min.	H_2	O_2	N_2	(min)	H_2	O_2	H_2	O_2
13	10	42	4.0	548594	119053	270520	0.00	7.70	16.51	22.49	11.28
13	20	44	14.0	807979	186599	193029	9.52	7.66	16.53	22.88	11.18
13	30	46	24.1	821262	191625	187136	19.56	7.62	16.55	23.30	11.07
13	40	50	34.1	818723	192489	187260	29.62	7.58	16.57	23.75	10.99
13	50	52	44.2	813480	192424	186834	39.66	7.55	16.60	24.06	10.81
14	0	56	54.2	807827	192468	186796	49.72	7.50	16.61	24.57	10.78
14	10	58	64.3	802432	192471	186831	59.76	7.45	16.60	25.09	10.79
14	21	2	74.3	797508	192741	186988	69.82	7.39	16.61	25.61	10.74
14	31	4	84.4	792593	192951	187195	79.86	7.34	16.61	26.15	10.74
14	41	8	94.4	787635	193081	187193	89.92	7.29	16.62	26.62	10.68
14	51	10	104.5	784018	193505	187570	99.96	7.25	16.63	27.10	10.67
15	1	14	114.5	779356	193519	187533	110.02	7.20	16.63	27.52	10.64
15	11	16	124.6	775898	193677	187459	120.06	7.18	16.65	27.81	10.53

$t_{correct.}$	Partial pressure (kPa)		Rate (mmol L^{-1} h^{-1})		d$[H_2O_2]$/dt	$\Sigma[H_2]$	$[H_2O_2]$	S_e	$\Sigma_2/[H_2O_2]$	$\Sigma_1/[H_2O_2]$
(min)	p_{H2}	p_{O2}	r_{H2}	r_{O2}	(mmol L^{-1} h^{-1})	(mmol L^{-1})	(mmol L^{-1})	(—)	(h)	(—)
0.00	17.08	36.61	19.96	18.74	17.52	0.00	0.00		0.000	0.000
9.52	17.00	36.66	20.31	18.57	16.84	3.19	2.73	0.85	0.079	1.172
19.56	16.92	36.72	20.67	18.40	16.12	6.62	5.48	0.83	0.165	1.208
29.62	16.83	36.78	21.07	18.26	15.44	10.12	8.13	0.80	0.251	1.245
39.66	16.76	36.85	21.35	17.97	14.59	13.67	10.64	0.78	0.340	1.285
49.72	16.66	36.91	21.81	17.91	14.01	17.29	13.04	0.75	0.429	1.326
59.76	16.57	36.95	22.27	17.93	13.60	20.98	15.35	0.73	0.520	1.367
69.82	16.47	37.00	22.73	17.85	12.97	24.75	17.57	0.71	0.611	1.408
79.86	16.37	37.05	23.21	17.85	12.49	28.59	19.70	0.69	0.703	1.451
89.92	16.28	37.10	23.62	17.75	11.88	32.52	21.75	0.67	0.797	1.495
99.96	16.19	37.15	24.05	17.72	11.40	36.51	23.69	0.65	0.892	1.541
110.02	16.11	37.19	24.42	17.68	10.94	40.57	25.57	0.63	0.988	1.587
120.06	16.05	37.24	24.68	17.50	10.33	44.68	27.35	0.61	1.086	1.634

H_2O_2 Synthesis Data Sheet

Entry No. 7 (Exp. G93) Employed in: Table 2

Catalyst, Additives			Reaction conditions		Gas feed rate (sccm)				
Name	Conc.	(Unit)	T_0 (℃)	8.2		H_2	O_2	N_2	Sum
Pd-PVP	8.33	(mg/L)	T (℃)	30.0	Set	10.00	20.00	20.00	50.00
			P_0 (hPa)	1006.7	Calibrated	9.98	18.63	19.88	48.50
			P (hPa)	1013.2	Determination of final $[H_2O_2]$		Sample (g)	Absorbance (—)	$[H_2O_2]$ (mmol L^{-1})
			Agitation (rpm)	1200					
							2.035	0.011	0.12
Comment: Catalyst activation: H_2 gas 20 sccm at 303 K for 40 min.					Analysis of H_2O_2 formation selectivity and H_2O_2 destruction rate			S_f (—)	0.0568
								k_d[Cat] (h^{-1})	0.1938
								R^2	0.9752

GC calibration		GC count			Ratio of sensitivity (toward N_2)				Feed gas measurement	
Timing	No.	H_2	O_2	N_2	H_2		O_2			
Before reaction	1	962461	196324	170438	0.0889	0.0889	0.814	0.813	T_a (℃)	14.0
	2	965009	196948	170696	0.0888		0.812		P_0 (hPa)	995.8
	3	965571	197035	171189	0.0890		0.814		Flow	(cc/min)
After reaction	4	969884	197872	171543	0.0888		0.812		H_2	10.85
	5	969999	197834	171485	0.0888		0.812		O_2	20.25
	6	969916	197867	171679	0.0889		0.813		N_2	21.61

Time				GC count			$t_{correct.}$	Outlet flow (sccm)		Conversion(%)	
H	M	S	min.	H_2	O_2	N_2	(min)	H_2	O_2	H_2	O_2
10	4	36	4.0	356038	109787	289721	0.00	3.70	15.31	62.92	17.83
10	14	40	14.1	434989	189563	220142	10.62	3.72	15.33	62.77	17.74
10	24	44	24.1	444127	199001	211854	20.68	3.73	15.34	62.63	17.67
10	34	48	34.2	446928	200239	210891	30.75	3.74	15.35	62.49	17.63
10	44	52	44.3	448236	200333	210472	40.82	3.76	15.38	62.31	17.43
10	54	56	54.3	449845	200367	210626	50.88	3.77	15.38	62.20	17.47
11	5	0	64.4	448306	199784	210005	60.95	3.77	15.38	62.22	17.47
11	15	4	74.5	450024	199948	209732	71.02	3.79	15.41	62.02	17.30
11	25	8	84.5	449684	200157	210377	81.08	3.78	15.38	62.17	17.46
11	35	12	94.6	449644	199669	209266	91.15	3.80	15.42	61.97	17.23
11	45	16	104.7	449553	199814	209919	101.22	3.78	15.39	62.10	17.42
11	55	20	114.7	449778	199914	209948	111.28	3.79	15.39	62.08	17.39
12	5	24	124.8	449933	199902	209919	121.35	3.79	15.39	62.07	17.39

$t_{correct.}$	Partial pressure (kPa)		Rate (mmol L^{-1} h^{-1})		d$[H_2O_2]$/dt	$\Sigma[H_2]$	$[H_2O_2]$	S_e	$\Sigma_2/[H_2O_2]$	$\Sigma_1/[H_2O_2]$
(min)	p_{H2}	p_{O2}	r_{H2}	r_{O2}	(mmol L^{-1} h^{-1})	(mmol L^{-1})	(mmol L^{-1})	(—)	(h)	(—)
0.00	9.24	38.21	56.09	29.66	3.23	0.00	0.00		0.000	0.000
10.62	9.27	38.22	55.95	29.52	3.09	9.91	0.56	0.06	0.088	17.743
20.68	9.30	38.23	55.82	29.39	2.96	19.29	1.07	0.06	0.174	18.093
30.75	9.33	38.23	55.70	29.33	2.96	28.64	1.56	0.05	0.260	18.333
40.82	9.36	38.27	55.54	28.99	2.45	37.98	2.02	0.05	0.350	18.840
50.88	9.39	38.24	55.44	29.07	2.70	47.29	2.45	0.05	0.442	19.322
60.95	9.38	38.25	55.46	29.06	2.67	56.59	2.90	0.05	0.528	19.529
71.02	9.42	38.28	55.28	28.77	2.26	65.88	3.31	0.05	0.619	19.895
81.08	9.39	38.24	55.41	29.05	2.69	75.16	3.73	0.05	0.709	20.171
91.15	9.43	38.29	55.24	28.66	2.08	84.45	4.13	0.05	0.800	20.465
101.22	9.41	38.25	55.35	28.99	2.62	93.72	4.52	0.05	0.890	20.731
111.28	9.41	38.25	55.34	28.94	2.54	103.01	4.95	0.05	0.973	20.793
121.35	9.41	38.25	55.32	28.93	2.53	112.29	5.38	0.05	1.057	20.875

H_2O_2 Synthesis Data Sheet

Entry No. 8 (Exp. T079) Employed in: Table 2

Catalyst, Additives			Reaction conditions		Gas feed rate (sccm)				
Name	Conc.	(Unit)	T_0 (℃)	27.6		H_2	O_2	N_2	Sum
Pt-PVP	8.36	(mg/L)	T (℃)	30.1	Set	10.00	20.00	20.00	50.00
			P_0 (hPa)	1003.9	Calibrated	10.10	18.49	20.23	48.82
			P (hPa)	1012.3	Determination of final $[H_2O_2]$		Sample (g)	Absorbance (—)	$[H_2O_2]$ (mmol L^{-1})
			Agitation (rpm)	1199					
							1.658	0.006	0.12
Comment: Catalyst activation: H_2 gas 20 sccm at 303 K for 40 min.					Analysis of H_2O_2 formation selectivity and H_2O_2 destruction rate			S_f (—)	0.4751
								k_d[Cat] (h^{-1})	0.0972
								R^2	0.4323

GC calibration		GC count			Ratio of sensitivity (toward N_2)				Feed gas measurement	
Timing	No.	H_2	O_2	N_2	H_2		O_2			
Before reaction	1	978197	193964	172963	0.0882	0.0881	0.815	0.814	T_a (℃)	27.2
	2	978267	194028	173088	0.0883		0.815		P_0 (hPa)	1005.5
	3	979482	193662	172867	0.0881		0.815		Flow	(cc/min)
After reaction	4	978665	193259	172422	0.0879		0.815		H_2	11.60
	5	978510	193982	172683	0.0880		0.813		O_2	21.24
	6	978822	193885	172643	0.0880		0.813		N_2	23.25

Time				GC count			$t_{correct.}$	Outlet flow (sccm)		Conversion(%)	
H	M	S	min.	H_2	O_2	N_2	(min)	H_2	O_2	H_2	O_2
14	52	6	4.0	713263	119074	245565	0.00	9.91	18.35	1.86	0.74
15	2	8	14.0	924076	183429	173198	9.94	9.91	18.35	1.80	0.72
15	12	12	24.1	935936	187741	168891	20.01	9.92	18.36	1.73	0.69
15	22	14	34.1	936540	187327	168182	30.04	9.93	18.36	1.69	0.70
15	32	16	44.2	936131	187200	167862	40.08	9.94	18.38	1.54	0.58
15	42	20	54.2	935471	186952	167759	50.14	9.94	18.37	1.55	0.65
15	52	22	64.3	935235	186995	167663	60.18	9.94	18.38	1.52	0.57
16	2	26	74.3	936382	187185	167806	70.24	9.95	18.38	1.48	0.55
16	12	28	84.4	936875	186961	167887	80.28	9.95	18.35	1.48	0.72
16	22	32	94.4	935869	187004	167576	90.34	9.95	18.39	1.40	0.51
16	32	34	104.5	935983	187034	167696	100.38	9.95	18.38	1.46	0.56
16	42	38	114.5	937081	187688	168041	110.44	9.94	18.41	1.55	0.42
16	52	40	124.6	937104	187804	168061	120.48	9.94	18.42	1.56	0.37

$t_{correct.}$	Partial pressure (kPa)		Rate (mmol L^{-1} h^{-1})		$d[H_2O_2]/dt$	$\Sigma[H_2]$	$[H_2O_2]$	S_e	$\Sigma_2/[H_2O_2]$	$\Sigma_1/[H_2O_2]$
(min)	p_{H2}	p_{O2}	r_{H2}	r_{O2}	(mmol L^{-1} h^{-1})	(mmol L^{-1})	(mmol L^{-1})	(—)	(h)	(—)
0.00	19.82	36.70	1.68	1.22	0.76	0.00	0.00		0.000	0.000
9.94	19.82	36.70	1.62	1.18	0.74	0.27	0.12	0.46	0.083	2.193
20.01	19.83	36.70	1.56	1.14	0.72	0.54	0.25	0.46	0.168	2.187
30.04	19.84	36.70	1.52	1.15	0.78	0.80	0.37	0.47	0.251	2.144
40.08	19.86	36.71	1.39	0.95	0.51	1.04	0.48	0.46	0.343	2.171
50.14	19.86	36.70	1.40	1.07	0.73	1.28	0.58	0.46	0.435	2.186
60.18	19.86	36.71	1.37	0.93	0.50	1.51	0.69	0.46	0.524	2.196
70.24	19.86	36.71	1.34	0.91	0.48	1.73	0.77	0.44	0.627	2.259
80.28	19.88	36.68	1.33	1.18	1.03	1.96	0.89	0.46	0.694	2.190
90.34	19.87	36.72	1.27	0.84	0.42	2.18	1.02	0.47	0.769	2.143
100.38	19.87	36.71	1.32	0.93	0.55	2.39	1.10	0.46	0.874	2.182
110.44	19.84	36.75	1.40	0.70	0.00	2.62	1.14	0.44	1.003	2.295
120.48	19.84	36.76	1.40	0.61	-0.18	2.85	1.13	0.39	1.185	2.533

H_2O_2 Synthesis Data Sheet

Entry No. 9 (Exp. T078) Employed in: Table 2

Catalyst, Additives			Reaction conditions		Gas feed rate (sccm)				
Name	Conc.	(Unit)	T_0 (℃)	27.4		H_2	O_2	N_2	Sum
Ru-PVP	8.36	(mg/L)	T (℃)	30.1	Set	10.00	20.00	20.00	50.00
			P_0 (hPa)	1004.8	Calibrated	10.10	18.49	20.23	48.82
H_2SO_4	0.01	(N)	P (hPa)	1013.2	Determination of final $[H_2O_2]$		Sample (g)	Absorbance (—)	$[H_2O_2]$ (mmol L^{-1})
NaBr	0.001	(N)	Agitation (rpm)	1201					
							1.676	0.031	0.64
Comment: Catalyst activation: H_2 gas 20 sccm at 303 K for 40 min.					Analysis of H_2O_2 formation selectivity and H_2O_2 destruction rate			S_f (—)	0.0893
								k_d[Cat] (h^{-1})	-0.6413
								R^2	0.8162

GC calibration		GC count			Ratio of sensitivity (toward N_2)				Feed gas measurement	
Timing	No.	H_2	O_2	N_2	H_2		O_2			
Before reaction	1	975780	193772	173493	0.0887	0.0883	0.818	0.817	T_a (℃)	27.2
	2	977695	193987	173624	0.0886		0.818		P_0 (hPa)	1005.5
	3	977621	193529	173203	0.0884		0.818		Flow	(cc/min)
After reaction	4	974601	192569	171816	0.0880		0.815		H_2	11.60
	5	974826	192525	171882	0.0880		0.816		O_2	21.24
	6	975100	192774	172118	0.0881		0.816		N_2	23.25

Time				GC count			$t_{correct.}$	Outlet flow (sccm)		Conversion(%)	
H	M	S	min.	H_2	O_2	N_2	(min)	H_2	O_2	H_2	O_2
10	45	18	4.0	650869	120683	249300	0.00	9.81	18.33	2.79	0.83
10	55	22	14.1	917093	183489	173815	9.97	9.83	18.34	2.60	0.78
11	5	24	24.1	931437	187000	168895	20.00	9.85	18.35	2.39	0.73
11	15	28	34.2	932130	187451	168608	30.07	9.88	18.37	2.18	0.62
11	25	30	44.2	931841	186908	168294	40.10	9.89	18.35	2.02	0.73
11	35	34	54.3	932287	186906	167944	50.17	9.92	18.39	1.77	0.52
11	45	36	64.3	930375	186392	167735	60.20	9.91	18.36	1.85	0.67
11	55	40	74.4	930979	186846	167864	70.27	9.91	18.39	1.86	0.51
12	5	42	84.4	930678	186257	167603	80.30	9.92	18.36	1.74	0.66
12	15	46	94.5	930617	186145	167538	90.37	9.92	18.36	1.71	0.69
12	25	48	104.5	930341	186061	167379	100.40	9.93	18.37	1.65	0.64
12	35	52	114.6	930916	186655	167555	110.47	9.92	18.41	1.69	0.42
12	45	54	124.6	931856	186869	167704	120.50	9.93	18.41	1.68	0.40

$t_{correct.}$	Partial pressure (kPa)		Rate (mmol L^{-1} h^{-1})		d$[H_2O_2]$/dt	$\Sigma[H_2]$	$[H_2O_2]$	S_e	$\Sigma_2/[H_2O_2]$	$\Sigma_1/[H_2O_2]$
(min)	p_{H2}	p_{O2}	r_{H2}	r_{O2}	(mmol L^{-1} h^{-1})	(mmol L^{-1})	(mmol L^{-1})	(—)	(h)	(—)
0.00	19.69	36.78	2.52	1.37	0.22	0.00	0.00		0.000	0.000
9.97	19.72	36.78	2.34	1.28	0.23	0.40	0.04	0.09	0.083	10.914
20.00	19.75	36.78	2.16	1.20	0.24	0.78	0.08	0.10	0.165	10.238
30.07	19.78	36.78	1.96	1.03	0.10	1.13	0.10	0.09	0.265	10.779
40.10	19.81	36.75	1.83	1.20	0.57	1.44	0.16	0.11	0.311	8.988
50.17	19.83	36.78	1.60	0.86	0.12	1.73	0.22	0.13	0.373	7.908
60.20	19.83	36.75	1.67	1.11	0.54	2.00	0.27	0.14	0.448	7.302
70.27	19.82	36.79	1.68	0.83	-0.01	2.28	0.32	0.14	0.541	7.163
80.30	19.85	36.74	1.57	1.10	0.62	2.56	0.37	0.14	0.622	6.911
90.37	19.85	36.73	1.54	1.13	0.72	2.82	0.48	0.17	0.625	5.839
100.40	19.86	36.74	1.49	1.05	0.62	3.07	0.59	0.19	0.659	5.168
110.47	19.84	36.79	1.52	0.70	-0.12	3.32	0.64	0.19	0.779	5.230
120.50	19.84	36.80	1.51	0.66	-0.20	3.58	0.61	0.17	0.984	5.880

H_2O_2 Synthesis Data Sheet

Entry No. 10 (Exp. T081) Employed in: Table 2

Catalyst, Additives			Reaction conditions		Gas feed rate (sccm)				
Name	Conc.	(Unit)	T_0 (℃)	28.4		H_2	O_2	N_2	Sum
Pt-PVP	8.36	(mg/L)	T (℃)	30.1	Set	10.00	20.00	20.00	50.00
			P_0 (hPa)	1005.1	Calibrated	10.10	18.49	20.23	48.82
			P (hPa)	1013.5	Determination of final $[H_2O_2]$		Sample (g)	Absorbance (—)	$[H_2O_2]$ (mmol L^{-1})
			Agitation (rpm)	1200					
							1.627	0.003	0.06
Comment: Catalyst activation: H_2 gas 20 sccm at 303 K for 40 min.					Analysis of H_2O_2 formation selectivity and H_2O_2 destruction rate			S_f (—)	-0.4808
								k_d[Cat] (h^{-1})	2.0549
								R^2	0.9910

GC calibration		GC count			Ratio of sensitivity (toward N_2)				Feed gas measurement	
Timing	No.	H_2	O_2	N_2	H_2		O_2			
Before reaction	1	979707	194167	173399	0.0883	0.0883	0.816	0.815	T_a (℃)	27.2
	2	980360	194446	173667	0.0884		0.816		P_0 (hPa)	1005.5
	3	980850	194313	173408	0.0882		0.815		Flow	(cc/min)
After reaction	4	979475	194182	173266	0.0883		0.815		H_2	11.60
	5	979768	194194	173312	0.0883		0.815		O_2	21.24
	6	979696	194086	173054	0.0881		0.815		N_2	23.25

Time				GC count			$t_{correct.}$	Outlet flow (sccm)		Conversion(%)	
H	M	S	min.	H_2	O_2	N_2	(min)	H_2	O_2	H_2	O_2
14	59	30	4.0	697304	118197	252905	0.00	9.98	18.45	1.10	0.18
15	9	34	14.1	931527	184559	174116	9.99	9.99	18.45	1.04	0.19
15	19	36	24.1	944908	188616	169341	20.02	10.00	18.45	0.99	0.20
15	29	40	34.2	945576	188746	168762	30.09	10.01	18.45	0.89	0.18
15	39	42	44.2	944381	188507	168682	40.12	10.00	18.44	0.96	0.26
15	49	46	54.3	944437	188280	168369	50.19	10.02	18.45	0.77	0.20
15	59	48	64.3	945381	188523	168640	60.22	10.01	18.44	0.84	0.23
16	9	52	74.4	942898	187971	168005	70.29	10.02	18.46	0.72	0.14
16	19	54	84.4	942372	187857	168106	80.32	10.01	18.44	0.84	0.26
16	29	58	94.5	943323	187995	168119	90.39	10.02	18.45	0.74	0.20
16	40	0	104.5	943262	187857	168015	100.42	10.03	18.45	0.69	0.21
16	50	4	114.6	943323	187983	168238	110.49	10.01	18.43	0.81	0.28
17	0	6	124.6	943765	187983	168222	120.52	10.02	18.44	0.76	0.27

$t_{correct.}$	Partial pressure (kPa)		Rate (mmol L^{-1} h^{-1})		d$[H_2O_2]$/dt	$\Sigma[H_2]$	$[H_2O_2]$	S_e	$\Sigma_2/[H_2O_2]$	$\Sigma_1/[H_2O_2]$
(min)	p_{H2}	p_{O2}	r_{H2}	r_{O2}	(mmol L^{-1} h^{-1})	(mmol L^{-1})	(mmol L^{-1})	(—)	(h)	(—)
0.00	19.92	36.81	0.99	0.30	-0.38	0.00	0.00		0.000	0.000
9.99	19.93	36.81	0.94	0.32	-0.31	0.16	-0.06	-0.36	0.083	-2.807
20.02	19.94	36.80	0.89	0.33	-0.23	0.31	-0.10	-0.33	0.177	-3.061
30.09	19.96	36.80	0.80	0.30	-0.20	0.46	-0.14	-0.30	0.276	-3.280
40.12	19.95	36.79	0.87	0.43	-0.01	0.59	-0.16	-0.26	0.403	-3.808
50.19	19.97	36.79	0.70	0.32	-0.05	0.73	-0.16	-0.22	0.556	-4.503
60.22	19.97	36.79	0.75	0.38	0.00	0.85	-0.17	-0.20	0.706	-5.112
70.29	19.98	36.80	0.65	0.24	-0.18	0.97	-0.18	-0.19	0.808	-5.340
80.32	19.97	36.78	0.75	0.44	0.12	1.08	-0.19	-0.17	0.952	-5.832
90.39	19.98	36.78	0.67	0.33	-0.02	1.20	-0.18	-0.15	1.170	-6.789
100.42	19.99	36.78	0.62	0.35	0.07	1.31	-0.17	-0.13	1.371	-7.603
110.49	19.97	36.77	0.73	0.45	0.18	1.42	-0.15	-0.11	1.739	-9.395
120.52	19.98	36.77	0.68	0.44	0.19	1.54	-0.12	-0.08	2.373	-12.785

H_2O_2 Synthesis Data Sheet

Entry No. 11 (Exp. T080) Employed in: Table 2

Catalyst, Additives			Reaction conditions		Gas feed rate (sccm)				
Name	Conc.	(Unit)	T_0 (℃)	28.8		H_2	O_2	N_2	Sum
Rh-PVP	8.31	(mg/L)	T (℃)	30.1	Set	10.00	20.00	20.00	50.00
			P_0 (hPa)	1005.8	Calibrated	10.12	18.41	20.24	48.77
H_2SO_4	0.01	(N)	P (hPa)	1014.1	Determination of final $[H_2O_2]$		Sample (g)	Absorbance (—)	$[H_2O_2]$ (mmol L^{-1})
NaBr	0.001	(N)	Agitation (rpm)	1199					
							1.681	0.044	0.90
Comment: Catalyst activation: H_2 gas 20 sccm at 303 K for 40 min.					Analysis of H_2O_2 formation selectivity and H_2O_2 destruction rate			S_f (—)	0.1167
								k_d[Cat] (h^{-1})	0.3794
								R^2	0.9239

GC calibration		GC count			Ratio of sensitivity (toward N_2)				Feed gas measurement	
Timing	No.	H_2	O_2	N_2	H_2		O_2			
Before reaction	1	980876	194282	174084	0.0887	0.0886	0.815	0.813	T_a (℃)	28.5
	2	982361	195102	174650	0.0889		0.814		P_0 (hPa)	1006.2
	3	982308	195075	174427	0.0887		0.813		Flow	(cc/min)
After reaction	4	979292	194274	173348	0.0885		0.811		H_2	11.70
	5	978960	194196	173328	0.0885		0.812		O_2	21.29
	6	978748	194241	173359	0.0885		0.812		N_2	23.41

Time				GC count			$t_{correct.}$	Outlet flow (sccm)		Conversion(%)	
H	M	S	min.	H_2	O_2	N_2	(min)	H_2	O_2	H_2	O_2
10	31	22	4.0	615460	120517	256558	0.00	9.57	18.10	5.44	1.66
10	41	26	14.1	899845	184585	176728	9.93	9.58	18.11	5.28	1.60
10	51	28	24.1	916482	188558	171761	19.96	9.60	18.12	5.11	1.55
11	1	32	34.2	917948	188715	171171	30.03	9.62	18.14	4.90	1.46
11	11	34	44.2	919379	188835	171398	40.06	9.62	18.13	4.88	1.53
11	21	38	54.3	918516	188371	170680	50.13	9.65	18.16	4.57	1.36
11	31	40	64.3	919509	188492	170706	60.16	9.66	18.17	4.48	1.31
11	41	44	74.4	918811	188173	170363	70.23	9.68	18.17	4.36	1.28
11	51	46	84.4	919550	188315	170445	80.26	9.68	18.18	4.33	1.25
12	1	50	94.5	920351	188370	170376	90.33	9.69	18.19	4.20	1.18
12	11	52	104.5	919670	188098	170182	100.36	9.69	18.19	4.17	1.21
12	21	56	114.6	920588	188260	170268	110.43	9.70	18.19	4.12	1.18
12	31	58	124.6	920720	188149	170056	120.46	9.71	18.20	3.99	1.11

$t_{correct.}$	Partial pressure (kPa)		Rate (mmol L^{-1} h^{-1})		$d[H_2O_2]/dt$	$\Sigma[H_2]$	$[H_2O_2]$	S_e	$\Sigma_2/[H_2O_2]$	$\Sigma_1/[H_2O_2]$
(min)	p_{H2}	p_{O2}	r_{H2}	r_{O2}	(mmol L^{-1} h^{-1})	(mmol L^{-1})	(mmol L^{-1})	(—)	(h)	(—)
0.00	19.40	36.71	4.92	2.72	0.53	0.00	0.00		0.000	0.000
9.93	19.42	36.71	4.77	2.64	0.51	0.80	0.09	0.11	0.083	9.379
19.96	19.45	36.71	4.62	2.55	0.49	1.59	0.17	0.11	0.168	9.413
30.03	19.47	36.72	4.42	2.40	0.38	2.34	0.24	0.10	0.260	9.725
40.06	19.48	36.70	4.40	2.51	0.62	3.08	0.32	0.11	0.339	9.493
50.13	19.52	36.72	4.12	2.23	0.34	3.80	0.41	0.11	0.422	9.369
60.16	19.53	36.72	4.04	2.15	0.26	4.48	0.46	0.10	0.534	9.837
70.23	19.55	36.72	3.94	2.10	0.27	5.15	0.50	0.10	0.647	10.307
80.26	19.55	36.72	3.91	2.06	0.20	5.81	0.54	0.09	0.761	10.772
90.33	19.57	36.73	3.80	1.94	0.09	6.45	0.56	0.09	0.892	11.448
100.36	19.58	36.72	3.76	1.99	0.22	7.08	0.59	0.08	1.016	12.014
110.43	19.58	36.72	3.72	1.94	0.15	7.71	0.62	0.08	1.128	12.420
120.46	19.60	36.73	3.60	1.83	0.06	8.32	0.64	0.08	1.263	13.043

H_2O_2 Synthesis Data Sheet

Entry No. 12 (Exp. Y276) Employed in: Table 2

Catalyst, Additives			Reaction conditions		Gas feed rate (sccm)				
Name	Conc.	(Unit)	T_0 (℃)	20.3		H_2	O_2	N_2	Sum
Ir-PVP	8.2	(mg/L)	T (℃)	29.8	Set	10.00	20.00	20.00	50.00
			P_0 (hPa)	1004.0	Calibrated	10.06	18.57	19.77	48.40
			P (hPa)	1012.2	Determination of final $[H_2O_2]$		Sample (g)	Absorbance (—)	$[H_2O_2]$ (mmol L^{-1})
			Agitation (rpm)	1205					
							1.455	0.005	0.12
Comment: Catalyst activation: H_2 gas 20 sccm at 303 K for 40 min.					Analysis of H_2O_2 formation selectivity and H_2O_2 destruction rate			S_f (—)	0.0630
								k_d[Cat] (h^{-1})	-0.0329
								R^2	0.0504

GC calibration		GC count			Ratio of sensitivity (toward N_2)				Feed gas measurement	
Timing	No.	H_2	O_2	N_2	H_2		O_2			
Before reaction	1	1007788	203036	175872	0.0888	0.0888	0.814	0.814	T_a (℃)	20.4
	2	1005525	202776	175518	0.0888		0.813		P_0 (hPa)	1003.2
	3	1005144	202857	175649	0.0889		0.813		Flow	(cc/min)
After reaction	4	1004429	202491	175450	0.0888		0.814		H_2	11.18
	5	1004519	202587	175483	0.0889		0.814		O_2	20.65
	6	1005535	202792	175583	0.0888		0.813		N_2	21.98

Time				GC count			$t_{correct.}$	Outlet flow (sccm)		Conversion(%)	
H	M	S	min.	H_2	O_2	N_2	(min)	H_2	O_2	H_2	O_2
15	5	18	4.0	708180	126364	254587	0.00	9.38	18.22	6.70	1.91
15	15	20	14.0	923377	193871	179863	10.24	9.41	18.23	6.42	1.84
15	25	24	24.1	938551	197928	175101	20.30	9.44	18.25	6.13	1.77
15	35	26	34.1	941906	198318	174740	30.34	9.47	18.26	5.87	1.71
15	45	30	44.2	943797	198262	174493	40.40	9.50	18.28	5.54	1.60
15	55	32	54.2	945775	198236	174413	50.44	9.52	18.28	5.30	1.57
16	5	36	64.3	951165	199147	174993	60.50	9.55	18.31	5.08	1.44
16	15	38	74.3	950767	198790	174648	70.54	9.56	18.31	4.93	1.43
16	25	42	84.4	951323	198692	174358	80.60	9.58	18.33	4.72	1.31
16	35	44	94.4	951744	198558	174314	90.64	9.59	18.32	4.65	1.35
16	45	48	104.5	952921	198891	174505	100.70	9.59	18.33	4.64	1.30
16	55	50	114.5	953218	198640	174320	110.74	9.60	18.33	4.51	1.32
17	5	52	124.6	953181	198599	174330	120.77	9.60	18.33	4.52	1.34

$t_{correct.}$	Partial pressure (kPa)		Rate (mmol L^{-1} h^{-1})		d$[H_2O_2]$/dt	$\Sigma[H_2]$	$[H_2O_2]$	S_e	$\Sigma_2/[H_2O_2]$	$\Sigma_1/[H_2O_2]$
(min)	p_{H2}	p_{O2}	r_{H2}	r_{O2}	(mmol L^{-1} h^{-1})	(mmol L^{-1})	(mmol L^{-1})	(—)	(h)	(—)
0.00	19.21	37.30	6.02	3.17	0.33	0.00	0.00		0.000	0.000
10.24	19.25	37.29	5.76	3.05	0.35	1.00	0.06	0.06	0.085	17.266
20.30	19.29	37.29	5.51	2.94	0.36	1.95	0.12	0.06	0.167	16.529
30.34	19.33	37.28	5.27	2.84	0.41	2.85	0.18	0.06	0.246	15.602
40.40	19.37	37.28	4.98	2.65	0.33	3.71	0.24	0.07	0.330	15.150
50.44	19.41	37.27	4.76	2.60	0.44	4.52	0.31	0.07	0.411	14.623
60.50	19.44	37.28	4.56	2.39	0.23	5.31	0.37	0.07	0.503	14.517
70.54	19.46	37.27	4.43	2.36	0.30	6.06	0.41	0.07	0.606	14.777
80.60	19.49	37.28	4.24	2.17	0.11	6.78	0.44	0.07	0.720	15.256
90.64	19.50	37.27	4.18	2.24	0.31	7.49	0.48	0.06	0.828	15.599
100.70	19.50	37.28	4.16	2.15	0.13	8.19	0.52	0.06	0.931	15.835
110.74	19.52	37.26	4.05	2.18	0.32	8.87	0.55	0.06	1.029	16.004
120.77	19.52	37.26	4.05	2.22	0.39	9.55	0.61	0.06	1.089	15.561

H_2O_2 Synthesis Data Sheet

Entry No. 13 (Exp. Y169) Employed in: Table 2

Catalyst, Additives			Reaction conditions		Gas feed rate (sccm)				
Name	Conc.	(Unit)	T_0 (℃)	20.8		H_2	O_2	N_2	Sum
Ir-PVP	8.17	(mg/L)	T (℃)	29.8	Set	10.00	20.00	20.00	50.00
			P_0 (hPa)	1006.4	Calibrated	9.89	18.69	19.82	48.41
H_2SO_4	0.01	(N)	P (hPa)	1014.4	Determination of final $[H_2O_2]$		Sample (g)	Absorbance (—)	$[H_2O_2]$ (mmol L^{-1})
NaBr	0.001	(N)	Agitation (rpm)	1204					
							1.013	0.016	0.53
Comment: Catalyst activation: H_2 gas 20 sccm at 303 K for 40 min.					Analysis of H_2O_2 formation selectivity and H_2O_2 destruction rate			S_f (—)	0.1375
								k_d[Cat] (h^{-1})	0.2161
								R^2	0.9512

GC calibration		GC count			Ratio of sensitivity (toward N_2)				Feed gas measurement	
Timing	No.	H_2	O_2	N_2	H_2		O_2			
Before reaction	1	996922	200785	174004	0.0871	0.0871	0.817	0.818	T_a (℃)	20.7
	2	996500	200673	174012	0.0872		0.817		P_0 (hPa)	1006.4
	3	996976	200780	173974	0.0871		0.817		Flow	(cc/min)
After reaction	4	999161	200593	174086	0.0870		0.818		H_2	10.98
	5	998063	200540	174138	0.0871		0.819		O_2	20.74
	6	997632	200420	173923	0.0870		0.818		N_2	22.00

Time				GC count			$t_{correct.}$	Outlet flow (sccm)		Conversion(%)	
H	M	S	min.	H_2	O_2	N_2	(min)	H_2	O_2	H_2	O_2
15	23	10	4.0	568472	123145	267227	0.00		17.46	21.83	6.59
15	33	12	14.0	809411	192400	189483	9.70	7.86	17.54	20.51	6.16
15	43	16	24.1	838255	197557	183033	19.77	8.00	17.62	19.13	5.71
15	53	18	34.1	852772	197666	181039	29.80	8.13	17.70	17.83	5.30
16	3	22	44.2	863215	197305	179643	39.87	8.29	17.80	16.17	4.73
16	13	24	54.2	872252	197360	179028	49.90	8.41	17.87	15.00	4.38
16	23	28	64.3	879998	197522	178595	59.97	8.50	17.93	14.04	4.07
16	33	30	74.3	885337	197732	178506	70.00	8.56	17.96	13.48	3.92
16	43	32	84.4	890060	197518	177942	80.03	8.63	17.99	12.74	3.72
16	53	36	94.4	893977	197691	177749	90.10	8.68	18.03	12.26	3.53
17	3	38	104.5	896849	197504	177437	100.13	8.72	18.04	11.82	3.45
17	13	42	114.5	898922	197486	177296	110.20	8.75	18.06	11.55	3.39
17	23	44	124.6	901751	197487	177346	120.23	8.78	18.05	11.30	3.41

$t_{correct.}$	Partial pressure (kPa)		Rate (mmol L^{-1} h^{-1})		$d[H_2O_2]/dt$	$\Sigma[H_2]$	$[H_2O_2]$	S_e	$\Sigma_2/[H_2O_2]$	$\Sigma_1/[H_2O_2]$
(min)	p_{H2}	p_{O2}	r_{H2}	r_{O2}	(mmol L^{-1} h^{-1})	(mmol L^{-1})	(mmol L^{-1})	(—)	(h)	(—)
0.00	16.69	37.68	19.28	10.99	2.70	0.00	0.00		0.000	0.000
9.70	16.90	37.68	18.12	10.28	2.44	3.02	0.42	0.14	0.081	7.280
19.77	17.11	37.68	16.90	9.53	2.16	5.96	0.80	0.13	0.169	7.441
29.80	17.31	37.67	15.75	8.84	1.93	8.69	1.14	0.13	0.261	7.603
39.87	17.55	37.68	14.29	7.90	1.51	11.21	1.43	0.13	0.359	7.829
49.90	17.73	37.67	13.25	7.31	1.37	13.51	1.67	0.12	0.463	8.079
59.97	17.87	37.67	12.40	6.79	1.18	15.67	1.89	0.12	0.569	8.306
70.00	17.95	37.66	11.91	6.54	1.18	17.70	2.08	0.12	0.674	8.496
80.03	18.07	37.65	11.25	6.21	1.16	19.64	2.28	0.12	0.776	8.616
90.10	18.13	37.66	10.83	5.89	0.95	21.49	2.46	0.11	0.882	8.748
100.13	18.20	37.64	10.45	5.76	1.08	23.27	2.63	0.11	0.987	8.859
110.20	18.24	37.64	10.20	5.65	1.09	25.00	2.81	0.11	1.085	8.901
120.23	18.29	37.61	9.98	5.69	1.41	26.69	3.02	0.11	1.171	8.844

H_2O_2 Synthesis Data Sheet

Entry No. 14 (Exp. T012) Employed in: Table 2 Fig. 9

Catalyst, Additives			Reaction conditions		Gas feed rate (sccm)				
Name	Conc.	(Unit)	T_0 (℃)	27.3		H_2	O_2	N_2	Sum
Pt-PVP	1.04	(mg/L)	T (℃)	30.2	Set	12.50	20.00	17.50	50.00
			P_0 (hPa)	1012.2	Calibrated	12.53	18.59	17.50	48.62
			P (hPa)	1019.1	Determination of final $[H_2O_2]$		Sample (g)	Absorbance (—)	$[H_2O_2]$ (mmol L^{-1})
			Agitation (rpm)	1199			1.315	0.018	0.47
Comment: Catalyst activation: H_2 gas 20 sccm at 303 K for 40 min.					Analysis of H_2O_2 formation selectivity and H_2O_2 destruction rate			S_f (—)	0.0416
								k_d[Cat] (h^{-1})	-0.0234
								R^2	0.4384

GC calibration		GC count			Ratio of sensitivity (toward N_2)				Feed gas measurement	
Timing	No.	H_2	O_2	N_2	H_2		O_2			
Before reaction	1	1252761	204639	156390	0.0893	0.0892	0.812	0.811	T_a (℃)	26.7
	2	1252197	204881	156415	0.0894		0.811		P_0 (hPa)	1012.5
	3	1251480	204979	156689	0.0896		0.812		Flow	(cc/min)
After reaction	4	1255132	204502	156061	0.0890		0.811		H_2	14.25
	5	1255064	204244	156133	0.0890		0.812		O_2	21.15
	6	1255501	204650	156299	0.0891		0.811		N_2	19.91

Time				GC count			$t_{correct.}$	Outlet flow (sccm)		Conversion(%)	
H	M	S	min.	H_2	O_2	N_2	(min)	H_2	O_2	H_2	O_2
10	53	16	4.0	652060	117398	269339	0.00	7.31	15.87	41.68	14.63
11	3	18	14.0	826618	194301	190376	9.14	7.40	15.92	40.93	14.37
11	13	22	24.1	858831	201859	181152	19.24	7.50	15.97	40.11	14.08
11	23	24	34.1	872071	202242	179225	29.24	7.60	16.03	39.32	13.80
11	33	28	44.2	880389	201777	178129	39.34	7.72	16.09	38.37	13.47
11	43	30	54.2	887031	201561	177408	49.34	7.81	16.13	37.65	13.21
11	53	34	64.3	891604	201418	176887	59.44	7.87	16.17	37.15	13.02
12	3	36	74.3	895675	201244	176477	69.44	7.93	16.19	36.71	12.89
12	13	38	84.4	898549	200930	176037	79.54	7.97	16.21	36.35	12.81
12	23	42	94.4	901167	201095	175919	89.54	8.00	16.23	36.12	12.68
12	33	44	104.5	903830	200775	175556	99.64	8.04	16.24	35.80	12.64
12	43	48	114.5	906666	200830	175424	109.64	8.07	16.26	35.55	12.55
12	53	50	124.6	908459	200760	175211	119.74	8.10	16.27	35.35	12.47

$t_{correct.}$	Partial pressure (kPa)		Rate (mmol L^{-1} h^{-1})		$d[H_2O_2]/dt$	$\Sigma[H_2]$	$[H_2O_2]$	S_e	$\Sigma_2/[H_2O_2]$	$\Sigma_1/[H_2O_2]$
(min)	p_{H2}	p_{O2}	r_{H2}	r_{O2}	(mmol L^{-1} h^{-1})	(mmol L^{-1})	(mmol L^{-1})	(—)	(h)	(—)
0.00	17.54	38.10	46.61	24.28	1.96	0.00	0.00		0.000	0.000
9.14	17.70	38.09	45.78	23.85	1.92	7.04	0.30	0.04	0.076	23.793
19.24	17.88	38.07	44.86	23.37	1.88	14.67	0.62	0.04	0.161	23.817
29.24	18.05	38.06	43.98	22.91	1.83	22.07	0.93	0.04	0.246	23.855
39.34	18.25	38.04	42.91	22.36	1.80	29.38	1.23	0.04	0.332	23.867
49.34	18.41	38.03	42.11	21.93	1.75	36.47	1.53	0.04	0.418	23.885
59.44	18.51	38.02	41.54	21.61	1.67	43.51	1.81	0.04	0.507	23.982
69.44	18.60	38.01	41.06	21.40	1.73	50.39	2.10	0.04	0.594	24.023
79.54	18.68	37.99	40.65	21.26	1.87	57.27	2.40	0.04	0.677	23.856
89.54	18.73	38.00	40.40	21.04	1.69	64.02	2.70	0.04	0.760	23.739
99.64	18.80	37.97	40.04	20.98	1.91	70.79	3.00	0.04	0.843	23.597
109.64	18.85	37.97	39.76	20.83	1.89	77.44	3.32	0.04	0.921	23.345
119.74	18.89	37.96	39.53	20.70	1.87	84.12	3.63	0.04	1.002	23.145

H_2O_2 Synthesis Data Sheet

Entry No. 15 (Exp. T028) Employed in: Table 2

Catalyst, Additives			Reaction conditions		Gas feed rate (sccm)				
Name	Conc.	(Unit)	T_0 (℃)	27.0		H_2	O_2	N_2	Sum
Pt-PVP	1.04	(mg/L)	T (℃)	30.2	Set	10.00	20.00	20.00	50.00
			P_0 (hPa)	1004.6	Calibrated	10.09	19.33	19.30	48.73
H_2SO_4	0.01	(N)	P (hPa)	1011.6	Determination of final $[H_2O_2]$		Sample (g)	Absorbance (—)	$[H_2O_2]$ (mmol L^{-1})
NaBr	0.001	(N)	Agitation (rpm)	1200					
							1.686	0.259	5.30
Comment: Catalyst activation: H_2 gas 20 sccm at 303 K for 40 min.					Analysis of H_2O_2 formation selectivity and H_2O_2 destruction rate			S_f (—)	0.1739
								k_d[Cat] (h^{-1})	0.3479
								R^2	0.9978

GC calibration		GC count			Ratio of sensitivity (toward N_2)				Feed gas measurement	
Timing	No.	H_2	O_2	N_2	H_2		O_2			
Before reaction	1	998058	200826	176724	0.0926	0.0923	0.881	0.881	T_a (℃)	27.3
	2	998170	200564	176434	0.0924		0.881		P_0 (hPa)	1003.9
	3	997827	200458	176387	0.0924		0.881		Flow	(cc/min)
After reaction	4	995137	199175	175394	0.0921		0.882		H_2	11.62
	5	996669	199389	175507	0.0920		0.881		O_2	22.26
	6	996476	199293	175418	0.0920		0.881		N_2	22.23

Time				GC count			$t_{correct.}$	Outlet flow (sccm)		Conversion(%)	
H	M	S	min.	H_2	O_2	N_2	(min)	H_2	O_2	H_2	O_2
17	12	2	4.0	449874	117752	277913	0.00	5.41	16.58	46.42	14.23
17	22	6	14.1	579386	188225	207894	9.28	5.42	16.61	46.28	14.08
17	32	8	24.1	600113	194487	200524	19.31	5.44	16.64	46.14	13.92
17	42	12	34.2	609354	195309	199354	29.38	5.44	16.67	46.05	13.78
17	52	14	44.2	610675	195022	198555	39.41	5.48	16.71	45.72	13.56
18	2	18	54.3	609714	195093	198383	49.48	5.47	16.73	45.76	13.45
18	12	20	64.3	608769	195230	198504	59.51	5.46	16.73	45.87	13.44
18	22	24	74.4	606211	195304	198559	69.58	5.44	16.73	46.11	13.43
18	32	26	84.4	604625	195570	198804	79.61	5.42	16.74	46.32	13.42
18	42	28	94.4	602168	195648	198921	89.65	5.39	16.73	46.57	13.44
18	52	32	104.5	599912	195344	198695	99.71	5.38	16.73	46.71	13.47
19	2	34	114.5	596488	195320	198783	109.75	5.34	16.72	47.04	13.52
19	12	38	124.6	597623	195367	198681	119.81	5.36	16.73	46.91	13.46

$t_{correct.}$	Partial pressure (kPa)		Rate (mmol L^{-1} h^{-1})		d$[H_2O_2]$/dt	$\Sigma[H_2]$	$[H_2O_2]$	S_e	$\Sigma_2/[H_2O_2]$	$\Sigma_1/[H_2O_2]$
(min)	p_{H2}	p_{O2}	r_{H2}	r_{O2}	(mmol L^{-1} h^{-1})	(mmol L^{-1})	(mmol L^{-1})	(—)	(h)	(—)
0.00	12.69	38.91	41.82	24.56	7.30	0.00	0.00		0.000	0.000
9.28	12.71	38.94	41.70	24.30	6.91	6.46	1.10	0.17	0.077	5.879
19.31	12.73	38.97	41.57	24.02	6.48	13.42	2.22	0.17	0.163	6.051
29.38	12.74	39.00	41.49	23.78	6.06	20.39	3.27	0.16	0.252	6.235
39.41	12.79	39.03	41.19	23.40	5.60	27.30	4.25	0.16	0.342	6.431
49.48	12.78	39.06	41.22	23.21	5.20	34.21	5.15	0.15	0.435	6.641
59.51	12.76	39.08	41.33	23.20	5.07	41.12	6.01	0.15	0.528	6.841
69.58	12.71	39.10	41.55	23.18	4.82	48.07	6.84	0.14	0.621	7.028
79.61	12.66	39.13	41.73	23.16	4.59	55.03	7.63	0.14	0.716	7.216
89.65	12.61	39.14	41.96	23.19	4.43	62.03	8.38	0.14	0.811	7.401
99.71	12.59	39.15	42.08	23.26	4.43	69.08	9.12	0.13	0.906	7.572
109.75	12.52	39.17	42.38	23.34	4.30	76.14	9.85	0.13	1.000	7.728
119.81	12.54	39.17	42.26	23.23	4.19	83.24	10.57	0.13	1.095	7.879

H_2O_2 Synthesis Data Sheet

Entry No. 16 (Exp. T077) Employed in: Table 2

Catalyst, Additives			Reaction conditions		Gas feed rate (sccm)				
Name	Conc.	(Unit)	T_0 (℃)	27.7		H_2	O_2	N_2	Sum
Au-PVP	8.33	(mg/L)	T (℃)	30.0	Set	10.00	20.00	20.00	50.00
			P_0 (hPa)	1005.2	Calibrated	10.11	18.24	20.23	48.58
			P (hPa)	1013.0	Determination of final $[H_2O_2]$		Sample (g)	Absorbance (—)	$[H_2O_2]$ (mmol L^{-1})
			Agitation (rpm)	1201					
							1.706	0.019	0.38
Comment: Catalyst activation: H_2 gas 20 sccm at 303 K for 40 min. Unsteady deactivation at early stage. Deleted from Fig. 2.					Analysis of H_2O_2 formation selectivity and H_2O_2 destruction rate			S_f (—)	2.4588
								k_d[Cat] (h^{-1})	0.2874
								R^2	0.9974

GC calibration		GC count			Ratio of sensitivity (toward N_2)				Feed gas measurement	
Timing	No.	H_2	O_2	N_2	H_2		O_2			
Before reaction	1	973343	193125	172933	0.0888	0.0888	0.807	0.807	T_a (℃)	29.2
	2	973929	193093	173075	0.0888		0.808		P_0 (hPa)	1007.0
	3	974150	193140	173042	0.0888		0.808		Flow	(cc/min)
After reaction	4	978115	193973	173554	0.0887		0.807		H_2	11.73
	5	977654	193879	173445	0.0887		0.807		O_2	21.16
	6	977045	193898	173554	0.0888		0.807		N_2	23.47

Time				GC count			$t_{correct.}$	Outlet flow (sccm)		Conversion(%)	
H	M	S	min.	H_2	O_2	N_2	(min)	H_2	O_2	H_2	O_2
16	10	38	4.0	703385	119786	245660	0.00	7.78	14.30	23.01	21.62
16	20	40	14.0	915094	183661	174590	9.67	8.17	15.00	19.22	17.73
16	30	44	24.1	927314	187450	169878	19.73	8.59	15.78	15.05	13.46
16	40	46	34.1	929783	187905	187905	29.77	8.88	16.33	12.13	10.46
16	50	50	44.2	928738	187740	169696	39.83	9.83	18.07	2.81	0.94
17	0	52	54.2	928864	187809	169586	49.87	9.83	18.08	2.73	0.84
17	10	56	64.3	929218	187787	169634	59.93	9.83	18.08	2.72	0.88
17	20	58	74.3	929259	187996	169787	69.97	9.83	18.08	2.81	0.86
17	31	2	84.4	927705	187681	169498	80.03	9.83	18.08	2.81	0.86
17	41	4	94.4	927417	187727	169513	90.07	9.82	18.08	2.84	0.84
17	51	8	104.5	925840	187368	169188	100.13	9.82	18.08	2.82	0.84
18	1	10	114.5	925440	187377	169110	110.17	9.83	18.09	2.82	0.79
18	11	14	124.6	928342	187730	169244	120.23	9.85	18.11	2.59	0.68

$t_{correct.}$	Partial pressure (kPa)		Rate (mmol L^{-1} h^{-1})		d$[H_2O_2]$/dt	$\Sigma[H_2]$	$[H_2O_2]$	S_f	$\Sigma_2/[H_2O_2]$	$\Sigma_1/[H_2O_2]$
(min)	p_{H2}	p_{O2}	r_{H2}	r_{O2}	(mmol L^{-1} h^{-1})	(mmol L^{-1})	(mmol L^{-1})	(—)	(h)	(—)
0.00	17.84	32.77	20.77	35.20	49.62	0.00	0.00		0.000	0.000
9.67	18.26	33.54	17.35	28.87	40.39	3.07	7.25	2.36	0.081	0.424
19.73	18.69	34.34	13.59	21.93	30.26	5.67	13.18	2.33	0.174	0.430
29.77	18.97	34.88	10.95	17.04	23.13	7.72	17.64	2.29	0.276	0.437
39.83	19.83	36.46	2.54	1.54	0.54	8.85	19.63	2.22	0.408	0.451
49.87	19.83	36.47	2.47	1.37	0.28	9.27	19.70	2.13	0.573	0.471
59.93	19.84	36.47	2.46	1.44	0.42	9.68	19.76	2.04	0.739	0.490
69.97	19.82	36.48	2.53	1.40	0.27	10.10	19.81	1.96	0.904	0.510
80.03	19.82	36.48	2.53	1.40	0.27	10.52	19.86	1.89	1.069	0.530
90.07	19.82	36.48	2.57	1.37	0.18	10.95	19.90	1.82	1.234	0.550
100.13	19.82	36.48	2.55	1.37	0.20	11.38	19.93	1.75	1.400	0.571
110.17	19.82	36.49	2.55	1.29	0.04	11.81	19.95	1.69	1.566	0.592
120.23	19.85	36.50	2.34	1.12	-0.11	12.22	19.94	1.63	1.734	0.613

H_2O_2 Synthesis Data Sheet

Entry No. 17 (Exp. T076) Employed in: Table 2

Catalyst, Additives			Reaction conditions		Gas feed rate (sccm)				
Name	Conc.	(Unit)	T_0 (℃)	29.1		H_2	O_2	N_2	Sum
Au-PVP	8.33	(mg/L)	T (℃)	30.1	Set	10.00	20.00	20.00	50.00
			P_0 (hPa)	1006.1	Calibrated	10.11	18.24	20.23	48.58
H_2SO_4	0.01	(N)	P (hPa)	1014.4	Determination of final $[H_2O_2]$		Sample (g)	Absorbance (—)	$[H_2O_2]$ (mmol L^{-1})
NaBr	0.001	(N)	Agitation (rpm)	1203					
							1.704	0.061	1.23
Comment: Catalyst activation: H_2 gas 20 sccm at 303 K for 40 min.					Analysis of H_2O_2 formation selectivity and H_2O_2 destruction rate			S_f (—)	-0.2610
								k_d[Cat] (h^{-1})	-0.5781
								R^2	0.9814

GC calibration		GC count			Ratio of sensitivity (toward N_2)				Feed gas measurement	
Timing	No.	H_2	O_2	N_2	H_2		O_2			
Before reaction	1	981158	194898	175181	0.0892	0.0890	0.810	0.814	T_a (℃)	29.2
	2	977883	186483	174220	0.0890		0.842		P_0 (hPa)	1007.0
	3	979394	194472	174623	0.0891		0.810		Flow	(cc/min)
After reaction	4	973343	193125	172933	0.0888		0.807		H_2	11.73
	5	973929	193093	173075	0.0888		0.808		O_2	21.16
	6	974150	193140	173042	0.0888		0.808		N_2	23.47

Time				GC count			$t_{correct.}$	Outlet flow (sccm)		Conversion(%)	
H	M	S	min.	H_2	O_2	N_2	(min)	H_2	O_2	H_2	O_2
12	40	46	4.0	642728	120737	250516	0.00	9.69	18.08	4.17	0.86
12	50	48	14.0	902565	182791	175013	9.90	9.71	18.09	3.98	0.79
13	0	52	24.1	917254	186502	170093	19.97	9.73	18.11	3.78	0.71
13	10	54	34.1	918679	186590	169600	30.00	9.75	18.12	3.58	0.64
13	20	58	44.2	919109	186432	169327	40.07	9.77	18.14	3.38	0.56
13	31	0	54.2	921122	186594	169351	50.10	9.79	18.15	3.18	0.49
13	41	2	64.3	920323	186407	168945	60.14	9.80	18.17	3.03	0.35
13	51	6	74.3	921140	186705	169161	70.20	9.80	18.18	3.07	0.32
14	1	8	84.4	921325	186740	169140	80.24	9.80	18.19	3.04	0.29
14	11	12	94.4	921747	186753	169173	90.30	9.81	18.18	3.01	0.30
14	21	14	104.5	919035	186062	168593	100.34	9.81	18.18	2.97	0.33
14	31	18	114.5	920460	186414	168613	110.40	9.82	18.21	2.83	0.15
14	41	20	124.6	922171	186758	169143	120.44	9.81	18.19	2.95	0.28

$t_{correct.}$	Partial pressure (kPa)		Rate (mmol L^{-1} h^{-1})		d$[H_2O_2]$/dt	$\Sigma[H_2]$	$[H_2O_2]$	S_e	$\Sigma_2/[H_2O_2]$	$\Sigma_1/[H_2O_2]$
(min)	p_{H2}	p_{O2}	r_{H2}	r_{O2}	(mmol L^{-1} h^{-1})	(mmol L^{-1})	(mmol L^{-1})	(—)	(h)	(—)
0.00	19.62	36.61	3.77	1.40	-0.96	0.00	0.00		0.000	0.000
9.90	19.65	36.62	3.59	1.28	-1.02	0.61	-0.16	-0.27	0.083	-3.700
19.97	19.67	36.62	3.41	1.16	-1.09	1.19	-0.34	-0.29	0.164	-3.502
30.00	19.70	36.62	3.23	1.04	-1.15	1.75	-0.53	-0.30	0.244	-3.316
40.07	19.73	36.62	3.05	0.92	-1.21	2.28	-0.73	-0.32	0.322	-3.139
50.10	19.75	36.62	2.87	0.80	-1.27	2.77	-0.93	-0.34	0.399	-2.972
60.14	19.77	36.64	2.74	0.58	-1.59	3.24	-1.17	-0.36	0.468	-2.767
70.20	19.76	36.65	2.77	0.52	-1.73	3.70	-1.45	-0.39	0.530	-2.555
80.24	19.76	36.66	2.74	0.47	-1.80	4.17	-1.74	-0.42	0.594	-2.388
90.30	19.77	36.65	2.72	0.49	-1.73	4.62	-2.04	-0.44	0.663	-2.266
100.34	19.78	36.64	2.68	0.54	-1.60	5.08	-2.32	-0.46	0.740	-2.188
110.40	19.79	36.68	2.55	0.25	-2.05	5.51	-2.63	-0.48	0.812	-2.099
120.44	19.78	36.65	2.67	0.46	-1.75	5.95	-2.94	-0.49	0.882	-2.021

H_2O_2 Synthesis Data Sheet

Entry No. 18 (Exp. T341) Employed in: Table 3 Fig. 6

Catalyst, Additives			Reaction conditions		Gas feed rate (sccm)				
Name	Conc.	(Unit)	T_0 (℃)	28.8		H_2	O_2	N_2	Sum
Pd-PVP	8.31	(mg/L)	T (℃)	30.1	Set	10.00	20.00	20.00	50.00
$Pt(NH_3)_4(NO_3)_2$	0.0833	(mg-Pt/L)	P_0 (hPa)	1010.3	Calibrated	10.06	18.03	20.30	48.39
H_2SO_4	0.01	(N)	P (hPa)	1016.5	Determination of final $[H_2O_2]$		Sample (g)	Absorbance (—)	$[H_2O_2]$ (mmol L^{-1})
NaBr	0.001	(N)	Agitation (rpm)	1200					
							0.420	0.561	46.04
Comment: Catalyst activation: H_2 gas 20 sccm at 303 K for 40 min.					Analysis of H_2O_2 formation selectivity and H_2O_2 destruction rate			S_f (—)	0.4774
								k_d[Cat] (h^{-1})	0.1894
								R^2	0.9864

GC calibration		GC count			Ratio of sensitivity (toward N_2)				Feed gas measurement	
Timing	No.	H_2	O_2	N_2	H_2		O_2			
Before reaction	1	1464950	294354	262893	0.0889	0.0892	0.793	0.793	T_a (℃)	29.0
	2	1474509	296356	264720	0.0890		0.793		P_0 (hPa)	1010.2
	3	1475699	296674	265319	0.0891		0.794		Flow	(cc/min)
After reaction	4	1613322	325883	291217	0.0894		0.793		H_2	11.62
	5	1617170	326632	291819	0.0894		0.793		O_2	20.82
	6	1634100	329939	294815	0.0894		0.793		N_2	23.45

Time				GC count			$t_{correct.}$	Outlet flow (sccm)		Conversion(%)	
H	M	S	min.	H_2	O_2	N_2	(min)	H_2	O_2	H_2	O_2
17	4	8	4.0	357093	92286	310691	0.00	3.71	13.32	63.15	26.13
17	14	12	14.1	449904	172347	238359	8.75	3.70	13.36	63.24	25.89
17	24	14	24.1	459388	186891	228679	18.78	3.69	13.41	63.34	25.62
17	34	18	34.2	468924	192634	230666	28.85	3.68	13.45	63.40	25.38
17	44	20	44.2	469941	195125	232565	38.88	3.66	13.51	63.62	25.03
17	54	24	54.3	469723	195471	232368	48.95	3.66	13.55	63.61	24.83
18	4	26	64.3	473146	197089	233820	58.98	3.66	13.58	63.57	24.68
18	14	30	74.4	477685	198821	235402	69.05	3.68	13.60	63.47	24.53
18	24	32	84.4	480342	199983	236370	79.08	3.68	13.63	63.42	24.40
18	34	34	94.4	474728	197594	233188	89.11	3.69	13.65	63.35	24.28
18	44	38	104.5	479665	199354	234773	99.18	3.70	13.68	63.22	24.13
18	54	40	114.5	482716	200363	235572	109.21	3.71	13.70	63.11	24.00
19	4	44	124.6	485877	201771	236679	119.28	3.72	13.73	63.04	23.82

$t_{correct.}$	Partial pressure (kPa)		Rate (mmol L^{-1} h^{-1})		$d[H_2O_2]/dt$	$\Sigma[H_2]$	$[H_2O_2]$	S_e	$\Sigma_2/[H_2O_2]$	$\Sigma_1/[H_2O_2]$
(min)	p_{H2}	p_{O2}	r_{H2}	r_{O2}	(mmol L^{-1} h^{-1})	(mmol L^{-1})	(mmol L^{-1})	(—)	(h)	(—)
0.00	9.68	34.75	56.72	42.05	27.39	0.00	0.00		0.000	0.000
8.75	9.64	34.83	56.80	41.67	26.55	8.28	3.93	0.48	0.073	2.105
18.78	9.61	34.92	56.89	41.24	25.59	17.78	8.29	0.47	0.158	2.145
28.85	9.58	35.00	56.95	40.84	24.74	27.33	12.51	0.46	0.244	2.184
38.88	9.51	35.13	57.15	40.28	23.42	36.87	16.54	0.45	0.332	2.229
48.95	9.51	35.18	57.14	39.97	22.80	46.46	20.42	0.44	0.420	2.276
58.98	9.51	35.23	57.10	39.72	22.35	56.01	24.19	0.43	0.509	2.315
69.05	9.53	35.26	57.01	39.48	21.95	65.58	27.91	0.43	0.598	2.350
79.08	9.53	35.30	56.96	39.27	21.58	75.11	31.55	0.42	0.686	2.381
89.11	9.54	35.32	56.90	39.08	21.26	84.63	35.13	0.42	0.775	2.409
99.18	9.57	35.36	56.79	38.83	20.87	94.17	38.66	0.41	0.864	2.436
109.21	9.59	35.39	56.69	38.63	20.56	103.66	42.13	0.41	0.954	2.461
119.28	9.59	35.43	56.63	38.34	20.06	113.16	45.54	0.40	1.044	2.485

H_2O_2 Synthesis Data Sheet

Entry No. 19 (Exp. T373) Employed in: Table 3

Catalyst, Additives			Reaction conditions		Gas feed rate (sccm)				
Name	Conc.	(Unit)	T_0 (℃)	23.4		H_2	O_2	N_2	Sum
Pd-PVP	8.29	(mg/L)	T (℃)	30.0	Set	10.00	20.00	20.00	50.00
$Pt(NH_3)_4(NO_3)_2$	0.0833	(mg-Pt/L)	P_0 (hPa)	998.9	Calibrated	10.25	18.24	19.81	48.29
H_2SO_4	0.01	(N)	P (hPa)	1004.9	Determination of final $[H_2O_2]$		Sample (g)	Absorbance (—)	$[H_2O_2]$ (mmol L^{-1})
NaBr	0.001	(N)	Agitation (rpm)	1200			0.712	1.086	52.61
Comment: Catalyst activation: H_2 gas 20 sccm at 303 K for 40 min. Treatment of activated catalyst: H_2 2 MPa at 303 K for 2 h.					Analysis of H_2O_2 formation selectivity and H_2O_2 destruction rate			S_f (—)	0.4477
								k_d[Cat] (h^{-1})	0.2009
								R^2	0.9838

GC calibration		GC count			Ratio of sensitivity (toward N_2)				Feed gas measurement	
Timing	No.	H_2	O_2	N_2	H_2		O_2			
Before reaction	1	1902305	386918	337988	0.0919	0.0920	0.804	0.805	T_a (℃)	23.7
	2	1920329	390884	341498	0.0920		0.804		P_0 (hPa)	996.8
	3	1923961	391468	341988	0.0920		0.804		Flow	(cc/min)
After reaction	4	1964178	399560	349133	0.0920		0.804		H_2	11.66
	5	1967996	400411	350548	0.0921		0.806		O_2	20.75
	6	1961158	398498	348265	0.0919		0.805		N_2	22.54

Time				GC count			$t_{correct.}$	Outlet flow (sccm)		Conversion(%)	
H	M	S	min.	H_2	O_2	N_2	(min)	H_2	O_2	H_2	O_2
15	19	10	4.0	361444	103076	370430	0.00	3.08	13.02	69.98	28.59
15	29	12	14.0	429561	200419	293358	8.55	3.05	13.06	70.22	28.38
15	39	16	24.1	462150	230357	289132	18.61	3.02	13.11	70.50	28.13
15	49	18	34.1	464516	231951	281093	28.65	3.01	13.15	70.62	27.88
15	59	22	44.2	434493	223290	269717	38.71	2.93	13.19	71.36	27.64
16	9	24	54.2	445080	228103	274546	48.75	2.95	13.24	71.18	27.38
16	19	26	64.3	447555	230196	276780	58.78	2.95	13.26	71.25	27.31
16	29	30	74.3	448611	230287	276337	68.85	2.96	13.28	71.14	27.16
16	39	32	84.4	450912	231221	276750	78.88	2.97	13.32	71.03	26.98
16	49	36	94.4	446896	228737	273315	88.95	2.98	13.34	70.93	26.85
16	59	38	104.5	447655	227921	271679	98.98	3.00	13.37	70.71	26.68
17	9	42	114.5	472348	234125	276583	109.05	3.11	13.49	69.64	26.02
17	19	44	124.6	494084	244774	288250	119.08	3.12	13.53	69.53	25.78

$t_{correct.}$	Partial pressure (kPa)		Rate (mmol L^{-1} h^{-1})		$d[H_2O_2]/dt$	$\Sigma[H_2]$	$[H_2O_2]$	S_e	$\Sigma_2/[H_2O_2]$	$\Sigma_1/[H_2O_2]$
(min)	p_{H2}	p_{O2}	r_{H2}	r_{O2}	(mmol L^{-1} h^{-1})	(mmol L^{-1})	(mmol L^{-1})	(—)	(h)	(—)
0.00	8.25	34.90	64.03	46.54	29.06	0.00	0.00		0.000	0.000
8.55	8.18	34.99	64.24	46.20	28.16	9.14	4.08	0.45	0.071	2.241
18.61	8.10	35.10	64.50	45.80	27.10	19.94	8.71	0.44	0.156	2.288
28.65	8.06	35.19	64.61	45.39	26.17	30.73	13.17	0.43	0.242	2.334
38.71	7.86	35.34	65.29	45.01	24.73	41.63	17.44	0.42	0.330	2.387
48.75	7.89	35.40	65.12	44.59	24.05	52.53	21.52	0.41	0.419	2.441
58.78	7.87	35.43	65.19	44.47	23.74	63.43	25.51	0.40	0.508	2.486
68.85	7.90	35.46	65.08	44.23	23.37	74.36	29.46	0.40	0.596	2.524
78.88	7.92	35.51	64.99	43.93	22.86	85.23	33.33	0.39	0.684	2.557
88.95	7.94	35.54	64.89	43.72	22.55	96.13	37.14	0.39	0.773	2.588
98.98	7.99	35.57	64.69	43.43	22.18	106.96	40.88	0.38	0.862	2.616
109.05	8.22	35.66	63.71	42.36	21.01	117.73	44.50	0.38	0.953	2.645
119.08	8.24	35.72	63.61	41.98	20.35	128.38	47.96	0.37	1.045	2.677

H_2O_2 Synthesis Data Sheet

Entry No. 20 (Exp. T381) Employed in: Table 3

Catalyst, Additives			Reaction conditions		Gas feed rate (sccm)				
Name	Conc.	(Unit)	T_0 (℃)	20.3		H_2	O_2	N_2	Sum
Pd-PVP	8.29	(mg/L)	T (℃)	29.9	Set	15.00	20.00	15.00	50.00
$Pt(NH_3)_4(NO_3)_2$	0.0833	(mg-Pt/L)	P_0 (hPa)	1003.2	Calibrated	15.09	18.55	14.51	48.15
H_2SO_4	0.01	(N)	P (hPa)	1007.9	Determination of final $[H_2O_2]$		Sample (g)	Absorbance (—)	$[H_2O_2]$ (mmol L^{-1})
NaBr	0.001	(N)	Agitation (rpm)	1198			0.447	0.936	72.26
Comment: Catalyst activation: H_2 gas 20 sccm at 303 K for 40 min. Treatment of activated catalyst: N_2 50 sccm at 343 K for 1 h.					Analysis of H_2O_2 formation selectivity and H_2O_2 destruction rate			S_f (—)	0.5450
								k_d[Cat] (h^{-1})	0.3540
								R^2	0.9945

GC calibration		GC count			Ratio of sensitivity (toward N_2)				Feed gas measurement	
Timing	No.	H_2	O_2	N_2	H_2		O_2			
Before reaction	1	2641683	374011	241549	0.0951	0.0955	0.826	0.826	T_a (℃)	18.5
	2	2683002	380350	245758	0.0953		0.826		P_0 (hPa)	1010.0
	3	2684227	380544	245748	0.0952		0.826		Flow	(cc/min)
After reaction	4	2928878	417318	269766	0.0958		0.826		H_2	16.51
	5	2880643	409785	264985	0.0957		0.827		O_2	20.29
	6	2966145	423029	273550	0.0959		0.827		N_2	15.87

Time				GC count			$t_{correct.}$	Outlet flow (sccm)		Conversion(%)	
H	M	S	min.	H_2	O_2	N_2	(min)	H_2	O_2	H_2	O_2
13	14	24	4.0	436705	73559	301053	0.00	4.07	10.00	73.06	46.06
13	24	26	14.0	590594	155274	239918	7.22	4.08	10.14	72.98	45.33
13	34	28	24.1	628996	181760	223011	17.25	4.09	10.33	72.87	44.30
13	44	32	34.1	629084	185833	211980	27.32	4.11	10.51	72.75	43.35
13	54	34	44.2	629641	189937	211586	37.35	4.12	10.76	72.68	41.99
14	4	38	54.2	621026	188825	207560	47.42	4.15	10.90	72.53	41.21
14	14	40	64.3	615895	189621	207128	57.45	4.12	10.97	72.70	40.84
14	24	44	74.3	630699	194538	210558	67.52	4.15	11.07	72.50	40.29
14	34	46	84.4	625935	195557	210681	77.55	4.12	11.13	72.72	40.01
14	44	50	94.4	635906	200070	214511	87.62	4.11	11.18	72.78	39.73
14	54	52	104.5	642829	202424	215710	97.65	4.13	11.25	72.64	39.36
15	4	56	114.5	634213	200226	212116	107.72	4.14	11.31	72.55	39.00
15	14	58	124.6	634780	201946	212961	117.75	4.13	11.37	72.63	38.72

$t_{correct.}$	Partial pressure (kPa)		Rate (mmol L^{-1} h^{-1})		d$[H_2O_2]$/dt	$\Sigma[H_2]$	$[H_2O_2]$	S_e	$\Sigma_2/[H_2O_2]$	$\Sigma_1/[H_2O_2]$
(min)	p_{H2}	p_{O2}	r_{H2}	r_{O2}	(mmol L^{-1} h^{-1})	(mmol L^{-1})	(mmol L^{-1})	(—)	(h)	(—)
0.00	13.74	33.80	98.44	76.27	54.10	0.00	0.00		0.000	0.000
7.22	13.70	34.08	98.34	75.06	51.78	11.84	6.37	0.54	0.060	1.858
17.25	13.66	34.47	98.19	73.35	48.51	28.27	14.76	0.52	0.146	1.916
27.32	13.63	34.83	98.03	71.78	45.53	44.73	22.65	0.51	0.233	1.975
37.35	13.55	35.35	97.93	69.53	41.13	61.12	29.89	0.49	0.324	2.045
47.42	13.54	35.62	97.73	68.24	38.75	77.53	36.59	0.47	0.417	2.119
57.45	13.44	35.79	97.96	67.63	37.29	93.89	42.95	0.46	0.510	2.186
67.52	13.48	35.96	97.69	66.72	35.76	110.31	49.08	0.44	0.604	2.247
77.55	13.36	36.11	97.99	66.26	34.54	126.67	54.96	0.43	0.697	2.305
87.62	13.31	36.23	98.07	65.79	33.50	143.12	60.67	0.42	0.792	2.359
97.65	13.34	36.34	97.88	65.17	32.47	159.50	66.18	0.41	0.886	2.410
107.72	13.35	36.46	97.76	64.58	31.40	175.91	71.54	0.41	0.981	2.459
117.75	13.29	36.58	97.87	64.12	30.36	192.27	76.70	0.40	1.077	2.507

H_2O_2 Synthesis Data Sheet

Entry No. 21 (Exp. T342) Employed in: Table 3 Fig. 6

Catalyst, Additives			Reaction conditions		Gas feed rate (sccm)				
Name	Conc.	(Unit)	T_0 (℃)	28.9		H_2	O_2	N_2	Sum
Pd-PVP	8.31	(mg/L)	T (℃)	30.1	Set	15.00	20.00	15.00	50.00
$Pt(NH_3)_4(NO_3)_2$	0.0833	(mg-Pt/L)	P_0 (hPa)	1008.7	Calibrated	15.07	18.42	15.13	48.62
H_2SO_4	0.01	(N)	P (hPa)	1014.1	Determination of final $[H_2O_2]$		Sample (g)	Absorbance (—)	$[H_2O_2]$ (mmol L^{-1})
NaBr	0.001	(N)	Agitation (rpm)	1200			0.626	1.237	68.11
Comment: Catalyst activation: H_2 gas 20 sccm at 303 K for 40 min.					Analysis of H_2O_2 formation selectivity and H_2O_2 destruction rate			S_f (—)	0.7215
								k_d[Cat] (h^{-1})	0.6178
								R^2	0.9956

GC calibration		GC count			Ratio of sensitivity (toward N_2)				Feed gas measurement	
Timing	No.	H_2	O_2	N_2	H_2		O_2			
Before reaction	1	1623170	221226	147983	0.0909	0.0922	0.814	0.816	T_a (℃)	25.8
	2	1757315	240464	160968	0.0913		0.815		P_0 (hPa)	1008.8
	3	1840509	252586	169016	0.0915		0.815		Flow	(cc/min)
After reaction	4	2355850	328331	220286	0.0932		0.817		H_2	17.13
	5	2350952	327922	220043	0.0933		0.817		O_2	20.93
	6	2349289	327613	219760	0.0932		0.817		N_2	17.19

Time				GC count			$t_{correct.}$	Outlet flow (sccm)		Conversion(%)	
H	M	S	min.	H_2	O_2	N_2	(min)	H_2	O_2	H_2	O_2
15	39	18	4.0	517368	79332	265463	0.00	6.67	11.20	55.72	39.17
15	49	20	14.0	844080	157109	201384	7.98	6.54	11.30	56.62	38.66
15	59	24	24.1	876927	176358	195787	18.04	6.37	11.41	57.74	38.02
16	9	26	34.1	867588	182385	195402	28.08	6.19	11.52	58.91	37.46
16	19	30	44.2	867248	189325	200094	38.14	6.05	11.68	59.89	36.60
16	29	32	54.2	844464	191518	201116	48.18	5.86	11.75	61.14	36.19
16	39	36	64.3	748978	196479	212361	58.24	4.92	11.42	67.36	38.01
16	49	38	74.3	759851	200758	215332	68.28	4.92	11.50	67.34	37.53
16	59	42	84.4	765726	201950	215252	78.34	4.96	11.58	67.08	37.14
17	9	44	94.4	767975	202517	214857	88.38	4.99	11.63	66.92	36.84
17	19	48	104.5	776531	204758	216141	98.44	5.01	11.69	66.75	36.53
17	29	50	114.5	770059	204322	215129	108.48	4.99	11.72	66.87	36.36
17	39	52	124.6	776457	206384	216248	118.51	5.01	11.78	66.77	36.05

$t_{correct.}$	Partial pressure (kPa)		Rate (mmol L^{-1} h^{-1})		$d[H_2O_2]/dt$	$\Sigma[H_2]$	$[H_2O_2]$	S_e	$\Sigma_2/[H_2O_2]$	$\Sigma_1/[H_2O_2]$
(min)	p_{H2}	p_{O2}	r_{H2}	r_{O2}	(mmol L^{-1} h^{-1})	(mmol L^{-1})	(mmol L^{-1})	(—)	(h)	(—)
0.00	19.65	32.98	74.99	64.41	53.83	0.00	0.00		0.000	0.000
7.98	19.28	33.30	76.20	63.57	50.95	10.05	6.96	0.69	0.066	1.443
18.04	18.81	33.70	77.71	62.52	47.33	22.96	15.21	0.66	0.153	1.510
28.08	18.33	34.08	79.29	61.60	43.91	36.09	22.84	0.63	0.241	1.580
38.14	17.88	34.54	80.60	60.19	39.77	49.50	29.86	0.60	0.332	1.658
48.18	17.38	34.88	82.29	59.52	36.75	63.12	36.26	0.57	0.426	1.741
58.24	15.19	35.25	90.66	62.50	34.34	77.63	42.22	0.54	0.522	1.839
68.28	15.15	35.42	90.63	61.72	32.80	92.79	47.83	0.52	0.618	1.940
78.34	15.22	35.52	90.28	61.07	31.86	107.96	53.26	0.49	0.714	2.027
88.38	15.26	35.60	90.07	60.59	31.11	123.04	58.52	0.48	0.810	2.103
98.44	15.30	35.68	89.84	60.06	30.28	138.13	63.67	0.46	0.905	2.170
108.48	15.23	35.76	90.00	59.79	29.59	153.17	68.68	0.45	1.000	2.230
118.51	15.25	35.85	89.86	59.28	28.70	168.21	73.55	0.44	1.096	2.287

H_2O_2 Synthesis Data Sheet

Entry No. 22 (Exp. T353) Employed in: Table 3

Catalyst, Additives			Reaction conditions		Gas feed rate (sccm)				
Name	Conc.	(Unit)	T_0 (℃)	28.4		H_2	O_2	N_2	Sum
Pd-PVP	8.29	(mg/L)	T (℃)	30.2	Set	15.00	20.00	15.00	50.00
$Pt(NH_3)_4(NO_3)_2$	0.0833	(mg-Pt/L)	P_0 (hPa)	1011.0	Calibrated	15.08	17.69	15.65	48.42
H_2SO_4	0.01	(N)	P (hPa)	1016.2	Determination of final $[H_2O_2]$		Sample (g)	Absorbance (—)	$[H_2O_2]$ (mmol L^{-1})
NaBr	0.001	(N)	Agitation (rpm)	1201			0.885	1.678	65.38
Comment: Catalyst activation: H_2 gas 20 sccm at 303 K for 40 min. Treatment of activated catalyst: N_2 50 sccm at 303 K for 1 h.					Analysis of H_2O_2 formation selectivity and H_2O_2 destruction rate			S_f (—)	0.6547
								k_d[Cat] (h^{-1})	0.7968
								R^2	0.9959

GC calibration		GC count			Ratio of sensitivity (toward N_2)				Feed gas measurement	
Timing	No.	H_2	O_2	N_2	H_2		O_2			
Before reaction	1	2160858	301480	202496	0.0903	0.0906	0.759	0.759	T_a (℃)	27.8
	2	2207723	308555	207346	0.0905		0.760		P_0 (hPa)	1010.9
	3	2246185	313995	210661	0.0904		0.758		Flow	(cc/min)
After reaction	4	2419752	339713	228171	0.0909		0.759		H_2	17.29
	5	2437349	342226	229709	0.0908		0.759		O_2	20.28
	6	2451258	344474	231150	0.0909		0.759		N_2	17.94

Time				GC count			$t_{correct.}$	Outlet flow (sccm)		Conversion(%)	
H	M	S	min.	H_2	O_2	N_2	(min)	H_2	O_2	H_2	O_2
12	48	2	4.0	539317	85785	305531	0.00	6.46	10.56	57.15	40.32
12	58	4	14.0	847764	166466	223223	7.80	6.22	10.61	58.77	40.01
13	8	8	24.1	847530	182485	209531	17.87	5.91	10.68	60.84	39.62
13	18	10	34.1	825019	189505	209841	27.90	5.58	10.73	63.03	39.37
13	28	14	44.2	789509	191793	209751	37.97	5.34	10.86	64.60	38.61
13	38	16	54.2	748956	195164	213465	48.00	4.98	10.86	67.00	38.62
13	48	20	64.3	621198	194988	220988	58.07	3.99	10.48	73.56	40.76
13	58	22	74.3	630449	198272	222582	68.10	4.02	10.58	73.36	40.19
14	8	26	84.4	643654	200758	222929	78.17	4.09	10.70	72.85	39.54
14	18	28	94.4	645706	200691	220965	88.20	4.14	10.79	72.52	39.02
14	28	32	104.5	651793	202679	221516	98.27	4.17	10.87	72.33	38.57
14	38	34	114.5	660072	205371	223078	108.30	4.20	10.93	72.17	38.19
14	48	38	124.6	661684	206657	223285	118.37	4.20	10.99	72.13	37.86

$t_{correct.}$	Partial pressure (kPa)		Rate (mmol L^{-1} h^{-1})		d$[H_2O_2]$/dt	$\Sigma[H_2]$	$[H_2O_2]$	S_e	$\Sigma_2/[H_2O_2]$	$\Sigma_1/[H_2O_2]$
(min)	p_{H2}	p_{O2}	r_{H2}	r_{O2}	(mmol L^{-1} h^{-1})	(mmol L^{-1})	(mmol L^{-1})	(—)	(h)	(—)
0.00	19.27	31.47	76.95	63.68	50.41	0.00	0.00		0.000	0.000
7.80	18.64	31.82	79.14	63.20	47.25	10.15	6.35	0.63	0.065	1.598
17.87	17.84	32.27	81.93	62.58	43.23	23.66	13.94	0.59	0.152	1.697
27.90	16.99	32.69	84.87	62.17	39.48	37.60	20.85	0.55	0.241	1.803
37.97	16.32	33.21	86.99	60.98	34.96	52.02	27.10	0.52	0.334	1.920
48.00	15.39	33.58	90.22	60.99	31.75	66.84	32.68	0.49	0.430	2.045
58.07	12.89	33.87	99.06	64.37	29.69	82.72	37.83	0.46	0.528	2.186
68.10	12.93	34.05	98.79	63.48	28.17	99.26	42.67	0.43	0.625	2.326
78.17	13.10	34.21	98.09	62.44	26.80	115.78	47.28	0.41	0.724	2.449
88.20	13.19	34.34	97.65	61.63	25.60	132.14	51.66	0.39	0.823	2.558
98.27	13.24	34.47	97.39	60.92	24.44	148.50	55.86	0.38	0.922	2.659
108.30	13.27	34.59	97.19	60.31	23.44	164.77	59.86	0.36	1.022	2.753
118.37	13.27	34.70	97.13	59.79	22.46	181.07	63.71	0.35	1.123	2.842

H_2O_2 Synthesis Data Sheet

Entry No. 23 (Exp. T359) Employed in: Table 3

Catalyst, Additives			Reaction conditions		Gas feed rate (sccm)				
Name	Conc.	(Unit)	T_0 (℃)	24.7		H_2	O_2	N_2	Sum
Pd-PVP	8.29	(mg/L)	T (℃)	30.1	Set	15.00	20.00	15.00	50.00
$Pt(NH_3)_4(NO_3)_2$	0.0833	(mg-Pt/L)	P_0 (hPa)	1011.7	Calibrated	14.94	18.46	14.80	48.20
H_2SO_4	0.01	(N)	P (hPa)	1017.0	Determination of final $[H_2O_2]$		Sample (g)	Absorbance (—)	$[H_2O_2]$ (mmol L^{-1})
NaBr	0.001	(N)	Agitation (rpm)	1200			0.684	1.260	63.46
Comment: Catalyst activation: H_2 gas 20 sccm at 303 K for 40 min. Treatment of activated catalyst: O_2 20 sccm, N_2 15 sccm at 303 K for 2 h.					Analysis of H_2O_2 formation selectivity and H_2O_2 destruction rate			S_f (—)	0.7384
								k_d[Cat] (h^{-1})	0.7810
								R^2	0.9965

GC calibration		GC count			Ratio of sensitivity (toward N_2)				Feed gas measurement	
Timing	No.	H_2	O_2	N_2	H_2		O_2			
Before reaction	1	1860428	257843	169779	0.0921	0.0933	0.822	0.823	T_a (℃)	24.7
	2	1909740	265264	174914	0.0925		0.823		P_0 (hPa)	1013.9
	3	2002438	278609	183576	0.0926		0.822		Flow	(cc/min)
After reaction	4	2448060	345601	228319	0.0942		0.824		H_2	16.79
	5	2476535	349756	230832	0.0941		0.823		O_2	20.75
	6	2502349	353496	233293	0.0941		0.823		N_2	16.63

Time				GC count			$t_{correct.}$	Outlet flow (sccm)		Conversion(%)	
H	M	S	min.	H_2	O_2	N_2	(min)	H_2	O_2	H_2	O_2
14	22	36	4.0	436033	110619	228715	0.00	6.81	11.40	54.38	38.23
14	32	38	14.0	769613	159707	191361	7.85	6.56	11.45	56.07	37.96
14	42	42	24.1	824878	172913	186585	17.92	6.24	11.52	58.21	37.61
14	52	44	34.1	820782	181498	190953	27.95	5.93	11.57	60.30	37.31
15	2	48	44.2	790015	185720	194022	38.02	5.62	11.66	62.39	36.87
15	12	50	54.2	765475	190757	198596	48.05	5.32	11.70	64.40	36.65
15	22	54	64.3	687186	193218	204238	58.12	4.64	11.52	68.92	37.60
15	32	56	74.3	668767	195782	205782	68.15	4.48	11.58	69.98	37.25
15	43	0	84.4	698505	202949	211219	78.22	4.56	11.70	69.45	36.63
15	53	2	94.4	713750	206520	213420	88.25	4.61	11.78	69.11	36.18
16	3	6	104.5	721689	207707	213229	98.32	4.67	11.86	68.74	35.75
16	13	8	114.5	728753	208338	212263	108.35	4.74	11.95	68.29	35.26
16	23	12	124.6	736748	209783	212282	118.42	4.79	12.03	67.94	34.82

$t_{correct.}$	Partial pressure (kPa)		Rate (mmol L^{-1} h^{-1})		d$[H_2O_2]$/dt	$\Sigma[H_2]$	$[H_2O_2]$	S_e	$\Sigma_2/[H_2O_2]$	$\Sigma_1/[H_2O_2]$
(min)	p_{H2}	p_{O2}	r_{H2}	r_{O2}	(mmol L^{-1} h^{-1})	(mmol L^{-1})	(mmol L^{-1})	(—)	(h)	(—)
0.00	20.12	33.67	72.54	63.01	53.49	0.00	0.00		0.000	0.000
7.85	19.49	34.02	74.79	62.56	50.34	9.64	6.80	0.70	0.065	1.419
17.92	18.69	34.48	77.64	62.00	46.36	22.43	14.91	0.66	0.152	1.505
27.95	17.89	34.92	80.42	61.50	42.58	35.64	22.34	0.63	0.241	1.595
38.02	17.07	35.42	83.21	60.77	38.33	49.37	29.13	0.59	0.333	1.695
48.05	16.29	35.83	85.89	60.41	34.93	63.51	35.26	0.56	0.428	1.801
58.12	14.61	36.25	91.92	61.98	32.04	78.43	40.87	0.52	0.525	1.919
68.15	14.16	36.57	93.34	61.40	29.46	93.92	46.02	0.49	0.624	2.041
78.22	14.31	36.70	92.63	60.37	28.11	109.52	50.85	0.46	0.725	2.154
88.25	14.41	36.80	92.17	59.63	27.09	124.97	55.46	0.44	0.825	2.253
98.32	14.53	36.89	91.68	58.93	26.19	140.39	59.93	0.43	0.925	2.343
108.35	14.66	36.99	91.08	58.13	25.18	155.67	64.22	0.41	1.025	2.424
118.42	14.76	37.08	90.62	57.40	24.17	170.92	68.36	0.40	1.125	2.500

H_2O_2 Synthesis Data Sheet

Entry No. 24 (Exp. T377) Employed in: Table 3

Catalyst, Additives			Reaction conditions		Gas feed rate (sccm)				
Name	Conc.	(Unit)	T_0 (℃)	22.1		H_2	O_2	N_2	Sum
Pd-PVP	8.29	(mg/L)	T (℃)	30.1	Set	15.00	20.00	15.00	50.00
$Pt(NH_3)_4(NO_3)_2$	0.0833	(mg-Pt/L)	P_0 (hPa)	1009.4	Calibrated	15.16	18.42	14.60	48.19
H_2SO_4	0.01	(N)	P (hPa)	1014.3	Determination of final $[H_2O_2]$		Sample (g)	Absorbance (—)	$[H_2O_2]$ (mmol L^{-1})
NaBr	0.001	(N)	Agitation (rpm)	1200					
							0.525	1.161	76.24
Comment: Catalyst activation: H_2 gas 20 sccm at 303 K for 40 min. Treatment of activated catalyst: N_2 50 sccm at 303 K for 2 h.					Analysis of H_2O_2 formation selectivity and H_2O_2 destruction rate			S_f (—)	0.9146
								k_d[Cat] (h^{-1})	1.0727
								R^2	0.9828

GC calibration		GC count			Ratio of sensitivity (toward N_2)				Feed gas measurement	
Timing	No.	H_2	O_2	N_2	H_2		O_2			
Before reaction	1	2395507	338432	218200	0.0946	0.0947	0.813	0.813	T_a (℃)	21.0
	2	2504099	354668	228637	0.0948		0.813		P_0 (hPa)	1011.9
	3	2515834	356331	229913	0.0949		0.814		Flow	(cc/min)
After reaction	4	2486073	351542	226652	0.0947		0.813		H_2	16.76
	5	2434911	343803	221721	0.0946		0.814		O_2	20.36
	6	2480777	350865	226167	0.0947		0.813		N_2	16.14

Time				GC count			$t_{correct.}$	Outlet flow (sccm)		Conversion(%)	
H	M	S	min.	H_2	O_2	N_2	(min)	H_2	O_2	H_2	O_2
14	28	44	4.0	514711	89772	329891	0.00	7.69	11.01	49.28	40.26
14	38	46	14.0	825686	167172	234427	7.52	7.03	10.95	53.64	40.58
14	48	50	24.1	902521	198318	230807	17.58	6.19	10.87	59.19	40.99
14	58	52	34.1	843287	199777	221195	27.62	5.27	10.73	65.23	41.76
15	8	56	44.2	761941	197886	216161	37.68	4.87	10.87	67.85	40.97
15	18	58	54.2	601527	194286	217696	47.72	3.82	10.60	74.80	42.45
15	29	0	64.3	601451	196133	217201	57.75	3.83	10.73	74.75	41.77
15	39	4	74.3	614875	200833	220691	67.82	3.85	10.81	74.59	41.32
15	49	6	84.4	610707	200040	218461	77.85	3.87	10.88	74.51	40.96
15	59	10	94.4	637773	208913	226553	87.92	3.89	10.95	74.33	40.54
16	9	12	104.5	632283	207269	223283	97.95	3.92	11.03	74.18	40.14
16	19	16	114.5	650399	213088	228143	108.02	3.94	11.09	74.00	39.77
16	29	18	124.6	649803	213656	227566	118.05	3.95	11.15	73.96	39.46

$t_{correct.}$	Partial pressure (kPa)		Rate (mmol L^{-1} h^{-1})		d$[H_2O_2]$/dt	$\Sigma[H_2]$	$[H_2O_2]$	S_e	$\Sigma_2/[H_2O_2]$	$\Sigma_1/[H_2O_2]$
(min)	p_{H2}	p_{O2}	r_{H2}	r_{O2}	(mmol L^{-1} h^{-1})	(mmol L^{-1})	(mmol L^{-1})	(—)	(h)	(—)
0.00	22.46	32.14	66.72	66.21	65.70	0.00	0.00		0.000	0.000
7.52	20.98	32.67	72.63	66.74	60.85	8.73	7.93	0.91	0.063	1.101
17.58	19.00	33.38	80.15	67.41	54.68	21.54	17.62	0.82	0.150	1.223
27.62	16.74	34.07	88.32	68.69	49.06	35.63	26.29	0.74	0.240	1.355
37.68	15.61	34.82	91.87	67.39	42.90	50.75	34.01	0.67	0.334	1.492
47.72	12.79	35.49	101.28	69.83	38.37	66.90	40.80	0.61	0.432	1.639
57.75	12.76	35.74	101.20	68.71	36.21	83.83	47.04	0.56	0.531	1.782
67.82	12.79	35.89	100.99	67.96	34.93	100.79	53.01	0.53	0.629	1.901
77.85	12.80	36.01	100.88	67.36	33.85	117.67	58.76	0.50	0.727	2.003
87.92	12.85	36.14	100.64	66.68	32.72	134.57	64.34	0.48	0.824	2.091
97.95	12.88	36.26	100.43	66.03	31.62	151.38	69.72	0.46	0.921	2.171
108.02	12.93	36.37	100.19	65.42	30.64	168.21	74.95	0.45	1.019	2.244
118.05	12.92	36.48	100.14	64.90	29.67	184.96	79.99	0.43	1.117	2.312

H_2O_2 Synthesis Data Sheet

Entry No. 25 (Exp. Y02) Employed in: Fig. 4 Fig. 5 Fig. 9 Fig. 10 Fig. 11

Catalyst, Additives			Reaction conditions		Gas feed rate (sccm)				
Name	Conc.	(Unit)	T_0 (℃)	22.8		H_2	O_2	N_2	Sum
Pd-PVP	8.33	(mg/L)	T (℃)	29.9	Set	10.00	20.00	20.00	50.00
			P_0 (hPa)	1006.6	Calibrated	10.20	18.55	19.86	48.60
H_2SO_4	0.01	(N)	P (hPa)	1014.0	Determination of final $[H_2O_2]$		Sample (g)	Absorbance (—)	$[H_2O_2]$ (mmol L^{-1})
NaBr	0.001	(N)	Agitation (rpm)	1200					
							0.672	0.541	27.55
Comment: Catalyst activation: H_2 gas 20 sccm at 303 K for 40 min.					Analysis of H_2O_2 formation selectivity and H_2O_2 destruction rate			S_f (—)	0.8753
								k_d[Cat] (h^{-1})	0.4713
								R^2	0.9998

GC calibration		GC count			Ratio of sensitivity (toward N_2)				Feed gas measurement	
Timing	No.	H_2	O_2	N_2	H_2		O_2			
Before reaction	1	966067	194223	171201	0.0910	0.0910	0.823	0.823	T_a (℃)	22.6
	2	966037	194091	171085	0.0909		0.823		P_0 (hPa)	1005.0
	3	966259	194222	171022	0.0909		0.822		Flow	(cc/min)
After reaction	4	965237	194114	170742	0.0908		0.822		H_2	11.44
	5	965596	194249	171215	0.0910		0.823		O_2	20.81
	6	968319	194966	171818	0.0911		0.823		N_2	22.28

Time				GC count			$t_{correct.}$	Outlet flow (sccm)		Conversion(%)	
H	M	S	min.	H_2	O_2	N_2	(min)	H_2	O_2	H_2	O_2
15	55	54	4.0	514854	105818	266719	0.00	7.79	16.30	23.63	12.13
16	5	58	14.1	766868	178028	190699	9.53	7.73	16.32	24.16	12.04
16	16	0	24.1	780060	183524	184524	19.56	7.68	16.33	24.72	11.94
16	26	4	34.2	777154	184354	184265	29.63	7.62	16.35	25.28	11.86
16	36	6	44.2	773085	185099	184689	39.66	7.56	16.38	25.84	11.71
16	46	10	54.3	769012	185601	185106	49.73	7.50	16.38	26.40	11.67
16	56	12	64.3	761274	185119	184286	59.76	7.46	16.41	26.82	11.51
17	6	16	74.4	755755	185544	185091	69.83	7.38	16.38	27.66	11.69
17	16	18	84.4	750658	185809	185117	79.86	7.32	16.40	28.16	11.57
17	26	22	94.5	744993	185973	185135	89.93	7.27	16.41	28.71	11.51
17	36	24	104.5	741576	186422	185491	99.96	7.22	16.42	29.17	11.46
17	46	28	114.6	737631	186625	185748	110.03	7.17	16.42	29.65	11.49
17	56	30	124.6	734368	186733	185444	120.06	7.15	16.45	29.84	11.29

$t_{correct.}$	Partial pressure (kPa)		Rate (mmol L^{-1} h^{-1})		$d[H_2O_2]/dt$	$\Sigma[H_2]$	$[H_2O_2]$	S_e	$\Sigma_2/[H_2O_2]$	$\Sigma_1/[H_2O_2]$
(min)	p_{H2}	p_{O2}	r_{H2}	r_{O2}	(mmol L^{-1} h^{-1})	(mmol L^{-1})	(mmol L^{-1})	(—)	(h)	(—)
0.00	17.22	36.04	21.51	20.08	18.66	0.00	0.00		0.000	0.000
9.53	17.11	36.11	21.99	19.93	17.87	3.45	2.90	0.84	0.079	1.191
19.56	17.00	36.18	22.51	19.77	17.04	7.17	5.82	0.81	0.165	1.233
29.63	16.89	36.25	23.02	19.64	16.27	10.99	8.61	0.78	0.252	1.276
39.66	16.78	36.33	23.53	19.39	15.25	14.88	11.25	0.76	0.341	1.323
49.73	16.67	36.39	24.03	19.32	14.61	18.87	13.75	0.73	0.431	1.372
59.76	16.58	36.47	24.41	19.05	13.69	22.93	16.12	0.70	0.523	1.422
69.83	16.43	36.49	25.18	19.36	13.53	27.09	18.40	0.68	0.615	1.472
79.86	16.33	36.56	25.64	19.17	12.70	31.34	20.60	0.66	0.708	1.521
89.93	16.22	36.63	26.14	19.05	11.97	35.68	22.67	0.64	0.803	1.574
99.96	16.13	36.68	26.56	18.98	11.40	40.08	24.62	0.61	0.900	1.628
110.03	16.04	36.71	26.99	19.02	11.06	44.58	26.50	0.59	0.998	1.682
120.06	15.99	36.78	27.17	18.70	10.23	49.10	28.28	0.58	1.097	1.736

H_2O_2 Synthesis Data Sheet

Entry No. 26 (Exp. Y23) Employed in: Fig. 4 Fig. 5 Fig. 9 Fig. 10 Fig. 11

Catalyst, Additives			Reaction conditions		Gas feed rate (sccm)				
Name	Conc.	(Unit)	T_0 (℃)	25.7		H_2	O_2	N_2	Sum
Pd-PVP	8.33	(mg/L)	T (℃)	30.2	Set	10.00	20.00	20.00	50.00
			P_0 (hPa)	994.0	Calibrated	10.12	18.43	20.19	
H_2SO_4	0.01	(N)	P (hPa)	1001.3	Determination of final $[H_2O_2]$		Sample (g)	Absorbance (—)	$[H_2O_2]$ (mmol L^{-1})
NaBr	0.001	(N)	Agitation (rpm)	1198					
							0.432	0.362	28.60
Comment: Catalyst activation: H_2 gas 20 sccm at 303 K for 40 min.					Analysis of H_2O_2 formation selectivity and H_2O_2 destruction rate			S_f (—)	0.8630
								k_d[Cat] (h^{-1})	0.5812
								R^2	0.9992

GC calibration		GC count			Ratio of sensitivity (toward N_2)				Feed gas measurement	
Timing	No.	H_2	O_2	N_2	H_2		O_2			
Before reaction	1	985816	196328	171127	0.0870	0.0869	0.795	0.796	T_a (℃)	24.9
	2	986350	196210	171099	0.0869		0.796		P_0 (hPa)	997.2
	3	986454	196241	171175	0.0870		0.796		Flow	(cc/min)
After reaction	4	984296	195839	170712	0.0869		0.796		H_2	11.58
	5	984637	195895	170702	0.0869		0.795		O_2	21.09
	6	984357	195928	170723	0.0869		0.795		N_2	23.11

Time				GC count			$t_{correct.}$	Outlet flow (sccm)		Conversion(%)	
H	M	S	min.	H_2	O_2	N_2	(min)	H_2	O_2	H_2	O_2
14	45	6	4.0	534208	116640	263574	0.00	7.68	16.17	24.07	12.22
14	55	8	14.0	777463	180210	189451	9.53	7.59	16.17	25.00	12.26
15	5	12	24.1	785398	185065	184795	19.60	7.49	16.16	25.98	12.30
15	15	14	34.1	777345	185613	184605	29.63	7.39	16.15	26.95	12.35
15	25	18	44.2	768096	185878	184874	39.70	7.29	16.15	27.93	12.35
15	35	20	54.2	759057	186009	185168	49.73	7.19	16.14	28.89	12.43
15	45	22	64.3	751110	186508	185598	59.77	7.10	16.14	29.80	12.40
15	55	26	74.3	741720	186590	185712	69.83	7.01	16.14	30.72	12.41
16	5	28	84.4	734063	186985	186251	79.87	6.92	16.13	31.63	12.48
16	15	32	94.4	726658	187340	186646	89.93	6.83	16.12	32.46	12.50
16	25	34	104.5	721204	187963	187345	99.97	6.76	16.12	33.22	12.54
16	35	68	115.0	715768	188355	187701	110.53	6.69	16.12	33.85	12.52
16	45	40	124.6	710799	188668	187899	120.07	6.64	16.13	34.38	12.47

$t_{correct.}$	Partial pressure (kPa)		Rate (mmol L^{-1} h^{-1})		$d[H_2O_2]/dt$	$\Sigma[H_2]$	$[H_2O_2]$	S_e	$\Sigma_2/[H_2O_2]$	$\Sigma_1/[H_2O_2]$
(min)	p_{H2}	p_{O2}	r_{H2}	r_{O2}	(mmol L^{-1} h^{-1})	(mmol L^{-1})	(mmol L^{-1})	(—)	(h)	(—)
0.00	16.73	35.22	21.74	20.10	18.46	0.00	0.00		0.000	0.000
9.53	16.56	35.28	22.58	20.17	17.75	3.52	2.88	0.82	0.079	1.224
19.60	16.38	35.35	23.47	20.23	16.99	7.38	5.79	0.78	0.165	1.275
29.63	16.21	35.42	24.35	20.32	16.29	11.38	8.57	0.75	0.252	1.328
39.70	16.03	35.50	25.23	20.32	15.42	15.54	11.23	0.72	0.340	1.383
49.73	15.85	35.55	26.10	20.45	14.81	19.83	13.76	0.69	0.429	1.441
59.77	15.68	35.64	26.92	20.40	13.88	24.26	16.16	0.67	0.520	1.502
69.83	15.51	35.71	27.75	20.42	13.10	28.85	18.42	0.64	0.614	1.566
79.87	15.34	35.77	28.57	20.54	12.50	33.56	20.56	0.61	0.709	1.632
89.93	15.19	35.83	29.32	20.57	11.81	38.42	22.60	0.59	0.805	1.700
99.97	15.04	35.89	30.01	20.63	11.25	43.38	24.53	0.57	0.902	1.768
110.53	14.92	35.94	30.58	20.60	10.63	48.71	26.46	0.54	1.006	1.841
120.07	14.82	36.00	31.05	20.52	9.98	53.61	28.10	0.52	1.102	1.908

H_2O_2 Synthesis Data Sheet

Entry No. 27 (Exp. Y46) Employed in: Fig. 4 Fig. 5 Fig. 9

Catalyst, Additives			Reaction conditions		Gas feed rate (sccm)				
Name	Conc.	(Unit)	T_0 (℃)	25.4		H_2	O_2	N_2	Sum
Pd-PVP	8.33	(mg/L)	T (℃)	30.2	Set	12.15	21.78	20.00	53.93
$Pt(NH_3)_4(NO_3)_2$	0.0167	(mg-Pt/L)	P_0 (hPa)	1002.6	Calibrated	12.22	20.03	20.42	52.67
H_2SO_4	0.01	(N)	P (hPa)	1010.3	Determination of final $[H_2O_2]$		Sample (g)	Absorbance (—)	$[H_2O_2]$ (mmol L^{-1})
NaBr	0.001	(N)	Agitation (rpm)	1198			0.568	0.590	35.60
Comment: Catalyst activation: H_2 gas 20 sccm at 303 K for 40 min.					Analysis of H_2O_2 formation selectivity and H_2O_2 destruction rate			S_f (—)	0.7827
								k_d[Cat] (h^{-1})	0.5836
								R^2	0.9999

GC calibration		GC count			Ratio of sensitivity (toward N_2)				Feed gas measurement	
Timing	No.	H_2	O_2	N_2	H_2		O_2			
Before reaction	1	1101665	197913	162014	0.0880	0.0879	0.803	0.803	T_a (℃)	25.3
	2	1104703	198135	162536	0.0881		0.804		P_0 (hPa)	1002.8
	3	1103656	197720	162065	0.0879		0.804		Flow	(cc/min)
After reaction	4	1100326	197011	161291	0.0877		0.803		H_2	13.94
	5	1100715	197064	161342	0.0877		0.803		O_2	22.84
	6	1100747	197068	161313	0.0877		0.803		N_2	23.29

Time				GC count			$t_{correct.}$	Outlet flow (sccm)		Conversion(%)	
H	M	S	min.	H_2	O_2	N_2	(min)	H_2	O_2	H_2	O_2
10	13	24	4.0	609414	120275	255689	0.00	8.38	16.62	31.45	17.03
10	23	28	14.1	837567	180839	186005	10.04	8.28	16.66	32.22	16.84
10	33	30	24.1	833645	185264	182636	20.07	8.19	16.70	33.00	16.64
10	43	34	34.2	823535	186206	182538	30.14	8.10	16.73	33.77	16.44
10	53	36	44.2	814549	186792	182680	40.17	8.00	16.77	34.55	16.25
11	3	40	54.3	806716	187624	183073	50.24	7.91	16.81	35.32	16.05
11	13	42	64.3	799247	188036	183205	60.27	7.83	16.84	35.96	15.93
11	23	46	74.4	791984	188651	183421	70.34	7.75	16.87	36.62	15.75
11	33	48	84.4	786381	189147	183855	80.37	7.67	16.88	37.21	15.73
11	43	52	94.5	780942	189335	183484	90.44	7.64	16.93	37.52	15.48
11	53	54	104.5	777336	189667	183437	100.47	7.60	16.96	37.80	15.31
12	3	58	114.6	774832	190158	183491	110.54	7.58	17.00	38.01	15.11
12	14	0	124.6	771868	190498	183503	120.57	7.55	17.03	38.26	14.97

$t_{correct.}$	Partial pressure (kPa)		Rate (mmol L^{-1} h^{-1})		d$[H_2O_2]$/dt	$\Sigma[H_2]$	$[H_2O_2]$	S_e	$\Sigma_2/[H_2O_2]$	$\Sigma_1/[H_2O_2]$
(min)	p_{H2}	p_{O2}	r_{H2}	r_{O2}	(mmol L^{-1} h^{-1})	(mmol L^{-1})	(mmol L^{-1})	(—)	(h)	(—)
0.00	17.86	35.41	34.32	30.46	26.59	0.00	0.00		0.000	0.000
10.04	17.68	35.54	35.17	30.10	25.04	5.81	4.32	0.74	0.084	1.346
20.07	17.50	35.67	36.02	29.75	23.49	11.77	8.38	0.71	0.170	1.404
30.14	17.32	35.79	36.86	29.41	21.95	17.88	12.19	0.68	0.258	1.467
40.17	17.13	35.92	37.70	29.05	20.40	24.11	15.73	0.65	0.349	1.533
50.24	16.95	36.05	38.54	28.71	18.87	30.51	19.02	0.62	0.441	1.604
60.27	16.80	36.14	39.25	28.49	17.72	37.01	22.08	0.60	0.536	1.676
70.34	16.65	36.26	39.96	28.17	16.38	43.66	24.95	0.57	0.633	1.750
80.37	16.52	36.32	40.62	28.13	15.65	50.40	27.62	0.55	0.730	1.824
90.44	16.43	36.42	40.95	27.68	14.40	57.24	30.14	0.53	0.830	1.899
100.47	16.36	36.49	41.25	27.37	13.50	64.11	32.48	0.51	0.932	1.974
110.54	16.30	36.57	41.49	27.03	12.57	71.05	34.66	0.49	1.035	2.050
120.57	16.23	36.63	41.75	26.77	11.78	78.01	36.70	0.47	1.141	2.126

H_2O_2 Synthesis Data Sheet

Entry No. 28 (Exp. Y54) Employed in: Fig. 4 Fig. 5 Fig. 9

Catalyst, Additives			Reaction conditions		Gas feed rate (sccm)				
Name	Conc.	(Unit)	T_0 (℃)	25.2		H_2	O_2	N_2	Sum
Pd-PVP	8.33	(mg/L)	T (℃)	30.1	Set	12.15	21.80	20.00	53.95
$Pt(NH_3)_4(NO_3)_2$	0.05	(mg-Pt/L)	P_0 (hPa)	1007.8	Calibrated	12.17	20.02	20.26	52.44
H_2SO_4	0.01	(N)	P (hPa)	1015.2	Determination of final $[H_2O_2]$		Sample (g)	Absorbance (—)	$[H_2O_2]$ (mmol L^{-1})
NaBr	0.001	(N)	Agitation (rpm)	1198					
							0.576	0.714	42.49
Comment: Catalyst activation: H_2 gas 20 sccm at 303 K for 40 min.					Analysis of H_2O_2 formation selectivity and H_2O_2 destruction rate			S_f (—)	0.7136
								k_d[Cat] (h^{-1})	0.4984
								R^2	0.9993

GC calibration		GC count			Ratio of sensitivity (toward N_2)				Feed gas measurement	
Timing	No.	H_2	O_2	N_2	H_2		O_2			
Before reaction	1	1106147	198082	162042	0.0880	0.0880	0.808	0.808	T_a (℃)	25.2
	2	1106340	198193	162030	0.0880		0.808		P_0 (hPa)	1007.0
	3	1106662	198190	162082	0.0880		0.808		Flow	(cc/min)
After reaction	4	1105712	198016	161836	0.0879		0.808		H_2	13.81
	5	1104875	197942	161745	0.0879		0.808		O_2	22.72
	6	1105017	197830	161733	0.0879		0.808		N_2	22.99

Time				GC count			$t_{correct.}$	Outlet flow (sccm)		Conversion(%)	
H	M	S	min.	H_2	O_2	N_2	(min)	H_2	O_2	H_2	O_2
18	59	0	4.0	578484	119664	261714	0.00	7.36	15.91	39.48	20.54
19	9	4	14.1	771077	180153	194249	10.18	7.27	15.96	40.23	20.28
19	19	6	24.1	765971	185244	190298	20.21	7.18	16.01	40.97	20.03
19	29	10	34.2	757843	186734	190353	30.28	7.09	16.06	41.71	19.80
19	39	12	44.2	748420	187520	190390	40.31	7.00	16.12	42.44	19.48
19	49	16	54.3	738395	187831	190272	50.38	6.91	16.16	43.18	19.29
19	59	18	64.3	730012	188370	190546	60.41	6.83	16.18	43.90	19.18
20	9	20	74.3	723342	189087	190937	70.44	6.75	16.21	44.53	19.04
20	19	24	84.4	717796	189437	190984	80.51	6.70	16.23	44.97	18.91
20	29	26	94.4	714061	189790	190918	90.54	6.66	16.27	45.24	18.73
20	39	30	104.5	711854	190413	191493	100.61	6.62	16.27	45.57	18.71
20	49	32	114.5	707251	190099	190369	110.64	6.62	16.34	45.60	18.36
20	59	36	124.6	704517	190308	190244	120.71	6.60	16.37	45.78	18.22

$t_{correct.}$	Partial pressure (kPa)		Rate (mmol L^{-1} h^{-1})		$d[H_2O_2]/dt$	$\Sigma[H_2]$	$[H_2O_2]$	S_e	$\Sigma_2/[H_2O_2]$	$\Sigma_1/[H_2O_2]$
(min)	p_{H2}	p_{O2}	r_{H2}	r_{O2}	(mmol L^{-1} h^{-1})	(mmol L^{-1})	(mmol L^{-1})	(—)	(h)	(—)
0.00	16.46	35.55	42.89	36.71	30.54	0.00	0.00		0.000	0.000
10.18	16.27	35.70	43.71	36.25	28.80	7.34	5.03	0.69	0.085	1.459
20.21	16.08	35.84	44.51	35.80	27.09	14.72	9.70	0.66	0.171	1.517
30.28	15.90	35.98	45.31	35.39	25.46	22.25	14.11	0.63	0.259	1.577
40.31	15.71	36.15	46.11	34.81	23.51	29.90	18.21	0.61	0.349	1.642
50.38	15.52	36.27	46.91	34.48	22.06	37.70	22.03	0.58	0.442	1.711
60.41	15.35	36.38	47.70	34.28	20.86	45.61	25.62	0.56	0.535	1.780
70.44	15.19	36.48	48.38	34.03	19.67	53.65	29.01	0.54	0.630	1.849
80.51	15.08	36.56	48.86	33.79	18.73	61.80	32.23	0.52	0.727	1.918
90.54	15.01	36.64	49.15	33.47	17.80	70.00	35.28	0.50	0.824	1.984
100.61	14.93	36.68	49.51	33.43	17.36	78.27	38.23	0.49	0.922	2.047
110.64	14.90	36.78	49.55	32.82	16.09	86.56	41.03	0.47	1.020	2.110
120.71	14.85	36.84	49.73	32.56	15.39	94.88	43.67	0.46	1.121	2.173

H_2O_2 Synthesis Data Sheet

Entry No. 29 (Exp. Y44) Employed in: Fig. 4 Fig. 5 Fig. 6 Fig. 9

Catalyst, Additives			Reaction conditions		Gas feed rate (sccm)				
Name	Conc.	(Unit)	T_0 (℃)	25.3		H_2	O_2	N_2	Sum
Pd-PVP	8.33	(mg/L)	T (℃)	30.1	Set	13.50	23.00	20.00	56.50
$Pt(NH_3)_4(NO_3)_2$	0.0833	(mg-Pt/L)	P_0 (hPa)	1001.8	Calibrated	13.62	21.16	20.37	55.15
H_2SO_4	0.01	(N)	P (hPa)	1009.2	Determination of final $[H_2O_2]$		Sample (g)	Absorbance (—)	$[H_2O_2]$ (mmol L^{-1})
NaBr	0.001	(N)	Agitation (rpm)	1200			0.512	0.789	52.82
Comment: Catalyst activation: H_2 gas 20 sccm at 303 K for 40 min.					Analysis of H_2O_2 formation selectivity and H_2O_2 destruction rate			S_f (—)	0.6468
								k_d[Cat] (h^{-1})	0.5017
								R^2	0.9964

GC calibration		GC count			Ratio of sensitivity (toward N_2)				Feed gas measurement	
Timing	No.	H_2	O_2	N_2	H_2		O_2			
Before reaction	1	1161740	198831	154690	0.0890	0.0889	0.808	0.808	T_a (℃)	25.5
	2	1161752	198787	154589	0.0890		0.808		P_0 (hPa)	1002.0
	3	1161271	198721	154608	0.0890		0.808		Flow	(cc/min)
After reaction	4	1161600	198398	154192	0.0888		0.808		H_2	15.56
	5	1161792	198496	154241	0.0888		0.807		O_2	24.18
	6	1161852	198501	154242	0.0888		0.807		N_2	23.27

Time				GC count			$t_{correct.}$	Outlet flow (sccm)		Conversion(%)	
H	M	S	min.	H_2	O_2	N_2	(min)	H_2	O_2	H_2	O_2
15	24	12	4.0	572374	120909	257597	0.00	7.47	16.09	45.17	23.98
15	34	14	14.0	745646	179909	194275	10.07	7.31	16.12	46.30	23.83
15	44	18	24.1	743416	185164	190051	20.14	7.16	16.15	47.43	23.68
15	54	20	34.1	733838	186575	189774	30.17	7.00	16.18	48.60	23.56
16	4	24	44.2	721645	187573	190145	40.24	6.87	16.23	49.55	23.30
16	14	26	54.2	706110	188344	190820	50.27	6.70	16.24	50.81	23.26
16	24	30	64.3	686126	188986	192145	60.34	6.46	16.18	52.53	23.53
16	34	32	74.3	663358	189592	193859	70.37	6.19	16.09	54.51	23.96
16	44	36	84.4	661915	190095	194281	80.44	6.17	16.10	54.71	23.93
16	54	38	94.4	668198	189782	192152	90.47	6.30	16.25	53.77	23.21
17	4	42	104.5	676341	190230	191352	100.54	6.40	16.36	53.01	22.71
17	14	44	114.5	681348	191151	191108	110.57	6.45	16.46	52.61	22.23
17	24	48	124.6	679165	191396	190934	120.64	6.44	16.49	52.71	22.06

$t_{correct.}$	Partial pressure (kPa)		Rate (mmol L^{-1} h^{-1})		$d[H_2O_2]/dt$	$\Sigma[H_2]$	$[H_2O_2]$	S_e	$\Sigma_2/[H_2O_2]$	$\Sigma_1/[H_2O_2]$
(min)	p_{H2}	p_{O2}	r_{H2}	r_{O2}	(mmol L^{-1} h^{-1})	(mmol L^{-1})	(mmol L^{-1})	(—)	(h)	(—)
0.00	16.44	35.41	54.93	45.32	35.71	0.00	0.00		0.000	0.000
10.07	16.14	35.58	56.30	45.03	33.76	9.33	5.83	0.62	0.084	1.601
20.14	15.85	35.75	57.67	44.74	31.81	18.89	11.33	0.60	0.170	1.668
30.17	15.54	35.92	59.09	44.52	29.95	28.66	16.49	0.58	0.258	1.737
40.24	15.28	36.10	60.25	44.03	27.82	38.67	21.34	0.55	0.348	1.812
50.27	14.95	36.25	61.78	43.95	26.12	48.87	25.85	0.53	0.440	1.891
60.34	14.53	36.37	63.87	44.46	25.05	59.41	30.14	0.51	0.533	1.971
70.37	14.04	36.47	66.28	45.28	24.27	70.29	34.27	0.49	0.626	2.051
80.44	13.98	36.50	66.52	45.21	23.90	81.43	38.31	0.47	0.719	2.126
90.47	14.18	36.61	65.38	43.86	22.33	92.46	42.17	0.46	0.813	2.193
100.54	14.34	36.67	64.46	42.90	21.35	103.35	45.84	0.44	0.909	2.255
110.57	14.42	36.76	63.96	42.01	20.06	114.09	49.30	0.43	1.006	2.314
120.64	14.38	36.83	64.10	41.69	19.28	124.83	52.60	0.42	1.106	2.373

H_2O_2 Synthesis Data Sheet

Entry No. 30 (Exp. Y49) Employed in: Fig. 4 Fig. 5 Fig. 9

Catalyst, Additives			Reaction conditions		Gas feed rate (sccm)				
Name	Conc.	(Unit)	T_0 (℃)	25.3		H_2	O_2	N_2	Sum
Pd-PVP	8.33	(mg/L)	T (℃)	30.4	Set	14.00	23.00	20.00	57.00
$Pt(NH_3)_4(NO_3)_2$	0.125	(mg-Pt/L)	P_0 (hPa)	1001.2	Calibrated	13.97	21.24	20.29	55.50
H_2SO_4	0.01	(N)	P (hPa)	1008.4	Determination of final $[H_2O_2]$		Sample (g)	Absorbance (—)	$[H_2O_2]$ (mmol L^{-1})
NaBr	0.001	(N)	Agitation (rpm)	1198			0.666	1.014	52.29
Comment: Catalyst activation: H_2 gas 20 sccm at 303 K for 40 min.					Analysis of H_2O_2 formation selectivity and H_2O_2 destruction rate			S_f (—)	0.4773
								k_d[Cat] (h^{-1})	0.1897
								R^2	1.0000

GC calibration		GC count			Ratio of sensitivity (toward N_2)				Feed gas measurement	
Timing	No.	H_2	O_2	N_2	H_2		O_2			
Before reaction	1	1200677	198450	153700	0.0882	0.0881	0.811	0.811	T_a (℃)	25.0
	2	1200414	198419	153752	0.0882		0.811		P_0 (hPa)	1000.2
	3	1200608	198358	153631	0.0881		0.811		Flow	(cc/min)
After reaction	4	1195314	197298	152710	0.0880		0.810		H_2	15.95
	5	1194923	197334	152725	0.0880		0.810		O_2	24.25
	6	1194077	197393	152789	0.0881		0.810		N_2	23.16

Time				GC count			$t_{correct.}$	Outlet flow (sccm)		Conversion(%)	
H	M	S	min.	H_2	O_2	N_2	(min)	H_2	O_2	H_2	O_2
18	25	14	4.0	571033	120471	260624	0.00	6.11	15.44	56.28	27.33
18	35	16	14.0	678618	180524	201727	10.97	6.10	15.49	56.36	27.08
18	45	20	24.1	673546	185883	197689	21.03	6.09	15.54	56.43	26.86
18	55	22	34.1	670361	186693	197022	31.07	6.08	15.58	56.47	26.63
19	5	26	44.2	665898	186659	196417	41.13	6.06	15.63	56.63	26.42
19	15	28	54.2	664541	186832	195965	51.17	6.06	15.68	56.62	26.18
19	25	32	64.3	663745	186999	195413	61.23	6.07	15.74	56.55	25.90
19	35	34	74.3	663756	187268	194974	71.27	6.08	15.80	56.45	25.63
19	45	38	84.4	663951	187524	194588	81.33	6.10	15.85	56.35	25.38
19	55	40	94.4	666901	188252	194420	91.37	6.13	15.93	56.12	25.03
20	5	44	104.5	667033	188525	194115	101.43	6.14	15.97	56.04	24.80
20	15	46	114.5	669002	188854	193694	111.47	6.17	16.04	55.81	24.50
20	25	48	124.6	670610	189242	193359	121.50	6.20	16.10	55.63	24.22

$t_{correct.}$	Partial pressure (kPa)		Rate (mmol L^{-1} h^{-1})		$d[H_2O_2]/dt$	$\Sigma[H_2]$	$[H_2O_2]$	S_e	$\Sigma_2/[H_2O_2]$	$\Sigma_1/[H_2O_2]$
(min)	p_{H2}	p_{O2}	r_{H2}	r_{O2}	(mmol L^{-1} h^{-1})	(mmol L^{-1})	(mmol L^{-1})	(—)	(h)	(—)
0.00	14.10	35.64	70.20	51.82	33.45	0.00	0.00		0.000	0.000
10.97	14.07	35.73	70.30	51.36	32.42	12.84	6.02	0.47	0.091	2.133
21.03	14.03	35.81	70.39	50.93	31.48	24.64	11.38	0.46	0.177	2.165
31.07	14.00	35.88	70.44	50.50	30.56	36.42	16.57	0.45	0.262	2.198
41.13	13.94	35.97	70.64	50.10	29.56	48.25	21.61	0.45	0.349	2.233
51.17	13.93	36.04	70.62	49.65	28.67	60.06	26.48	0.44	0.437	2.268
61.23	13.93	36.11	70.54	49.12	27.71	71.90	31.21	0.43	0.526	2.304
71.27	13.94	36.19	70.41	48.61	26.80	83.69	35.76	0.43	0.615	2.340
81.33	13.95	36.25	70.29	48.13	25.98	95.49	40.19	0.42	0.706	2.376
91.37	13.99	36.33	70.00	47.46	24.92	107.22	44.45	0.41	0.798	2.412
101.43	13.99	36.39	69.90	47.03	24.16	118.96	48.56	0.41	0.891	2.450
111.47	14.03	36.45	69.62	46.47	23.32	130.62	52.53	0.40	0.984	2.486
121.50	14.06	36.52	69.39	45.93	22.46	142.25	56.36	0.40	1.079	2.524

H_2O_2 Synthesis Data Sheet

Entry No. 31 (Exp. Y53) Employed in: Fig. 4 Fig. 5 Fig. 9

Catalyst, Additives			Reaction conditions		Gas feed rate (sccm)				
Name	Conc.	(Unit)	T_0 (℃)	25.6		H_2	O_2	N_2	Sum
Pd-PVP	8.33	(mg/L)	T (℃)	30.2	Set	15.50	24.50	20.00	60.00
$Pt(NH_3)_4(NO_3)_2$	0.125	(mg-Pt/L)	P_0 (hPa)	1006.8	Calibrated	15.61	22.63	20.27	58.50
H_2SO_4	0.01	(N)	P (hPa)	1014.5	Determination of final $[H_2O_2]$		Sample (g)	Absorbance (—)	$[H_2O_2]$ (mmol L^{-1})
NaBr	0.001	(N)	Agitation (rpm)	1201			0.459	0.774	57.79
Comment: Catalyst activation: H_2 gas 20 sccm at 303 K for 40 min.					Analysis of H_2O_2 formation selectivity and H_2O_2 destruction rate			S_f (—)	0.6120
								k_d[Cat] (h^{-1})	0.5093
								R^2	0.9891

GC calibration		GC count			Ratio of sensitivity (toward N_2)				Feed gas measurement	
Timing	No.	H_2	O_2	N_2	H_2		O_2			
Before reaction	1	1252567	200979	146253	0.0899	0.0898	0.812	0.813	T_a (℃)	25.5
	2	1252841	200777	146158	0.0898		0.813		P_0 (hPa)	1006.6
	3	1252302	200738	146067	0.0898		0.812		Flow	(cc/min)
After reaction	4	1252071	200577	145967	0.0898		0.812		H_2	17.75
	5	1251961	200671	146212	0.0899		0.813		O_2	25.73
	6	1253935	200915	146206	0.0898		0.812		N_2	23.05

Time				GC count			$t_{correct.}$	Outlet flow (sccm)		Conversion(%)	
H	M	S	min.	H_2	O_2	N_2	(min)	H_2	O_2	H_2	O_2
14	53	28	4.0	624891	124674	251722	0.00	8.59	16.91	44.97	25.25
15	3	30	14.0	796545	182321	189011	9.91	8.29	16.88	46.88	25.42
15	13	34	24.1	793019	187345	185236	19.98	7.99	16.84	48.79	25.58
15	23	36	34.1	780148	188747	185154	30.01	7.67	16.79	50.84	25.80
15	33	40	44.2	763958	190015	186390	40.08	7.46	16.79	52.18	25.79
15	43	42	54.2	732179	190616	187791	50.11	7.10	16.72	54.51	26.12
15	53	46	64.3	707549	191041	189227	60.18	6.81	16.63	56.37	26.51
16	3	48	74.3	714871	191642	188525	70.21	6.91	16.74	55.76	26.01
16	13	52	84.4	727001	191997	187070	80.28	7.08	16.90	54.66	25.29
16	23	54	94.4	743721	192422	185160	90.31	7.31	17.12	53.14	24.36
16	33	56	104.5	753886	192975	183963	100.35	7.46	17.28	52.19	23.64
16	44	0	114.5	752626	193379	183816	110.41	7.46	17.33	52.23	23.42
16	54	2	124.6	747189	193767	184197	120.45	7.39	17.33	52.67	23.43

$t_{correct.}$	Partial pressure (kPa)		Rate (mmol L^{-1} h^{-1})		d$[H_2O_2]$/dt	$\Sigma[H_2]$	$[H_2O_2]$	S_e	$\Sigma_2/[H_2O_2]$	$\Sigma_1/[H_2O_2]$
(min)	p_{H2}	p_{O2}	r_{H2}	r_{O2}	(mmol L^{-1} h^{-1})	(mmol L^{-1})	(mmol L^{-1})	(—)	(h)	(—)
0.00	18.24	35.92	62.68	51.01	39.34	0.00	0.00		0.000	0.000
9.91	17.74	36.11	65.34	51.34	37.35	10.58	6.34	0.60	0.083	1.669
19.98	17.23	36.29	68.00	51.68	35.36	21.76	12.44	0.57	0.169	1.750
30.01	16.67	36.48	70.85	52.12	33.38	33.37	18.18	0.54	0.256	1.835
40.08	16.29	36.65	72.72	52.11	31.50	45.42	23.63	0.52	0.346	1.922
50.11	15.65	36.85	75.97	52.76	29.55	57.85	28.73	0.50	0.437	2.013
60.18	15.14	36.97	78.57	53.56	28.56	70.81	33.60	0.47	0.529	2.107
70.21	15.28	37.05	77.71	52.54	27.37	83.88	38.28	0.46	0.621	2.191
80.28	15.54	37.13	76.17	51.10	26.02	96.79	42.76	0.44	0.715	2.264
90.31	15.91	37.22	74.05	49.20	24.35	109.35	46.97	0.43	0.811	2.328
100.35	16.12	37.31	72.73	47.77	22.80	121.62	50.91	0.42	0.909	2.389
110.41	16.09	37.38	72.79	47.32	21.85	133.83	54.66	0.41	1.009	2.448
120.45	15.96	37.44	73.41	47.33	21.25	146.05	58.26	0.40	1.108	2.507

H_2O_2 Synthesis Data Sheet

Entry No. 32 (Exp. Y45) Employed in: Fig. 4 Fig. 5 Fig. 9

Catalyst, Additives			Reaction conditions		Gas feed rate (sccm)				
Name	Conc.	(Unit)	T_0 (℃)	25.7		H_2	O_2	N_2	Sum
Pd-PVP	8.33	(mg/L)	T (℃)	30.4	Set	14.30	22.70	20.00	57.00
$Pt(NH_3)_4(NO_3)_2$	0.1667	(mg-Pt/L)	P_0 (hPa)	1002.8	Calibrated	14.33	20.89	20.22	55.44
H_2SO_4	0.01	(N)	P (hPa)	1009.9	Determination of final $[H_2O_2]$		Sample (g)	Absorbance (—)	$[H_2O_2]$ (mmol L^{-1})
NaBr	0.001	(N)	Agitation (rpm)	1200			0.566	0.926	56.18
Comment: Catalyst activation: H_2 gas 20 sccm at 303 K for 40 min.					Analysis of H_2O_2 formation selectivity and H_2O_2 destruction rate			S_f (—)	0.4376
								k_d[Cat] (h^{-1})	0.1461
								R^2	0.9998

GC calibration		GC count			Ratio of sensitivity (toward N_2)				Feed gas measurement	
Timing	No.	H_2	O_2	N_2	H_2		O_2			
Before reaction	1	1217558	194720	153168	0.0891	0.0891	0.812	0.812	T_a (℃)	25.5
	2	1218073	194765	153217	0.0891		0.813		P_0 (hPa)	1002.2
	3	1218007	194719	153218	0.0891		0.813		Flow	(cc/min)
After reaction	4	1219218	195050	153281	0.0891		0.812		H_2	16.37
	5	1218415	194811	153009	0.0890		0.811		O_2	23.86
	6	1218069	194729	152989	0.0890		0.811		N_2	23.10

Time				GC count			$t_{correct.}$	Outlet flow (sccm)		Conversion(%)	
H	M	S	min.	H_2	O_2	N_2	(min)	H_2	O_2	H_2	O_2
19	49	18	4.0	573679	117108	261580	0.00	5.99	14.89	58.21	28.69
19	59	22	14.1	663483	176758	204789	11.06	6.00	14.95	58.15	28.44
20	9	24	24.1	664992	182326	200986	21.09	6.01	14.99	58.09	28.22
20	19	28	34.2	665309	182563	199347	31.16	6.01	15.04	58.04	28.00
20	29	30	44.2	665005	182803	198932	41.19	6.02	15.09	57.98	27.76
20	39	32	54.2	665246	183210	198807	51.23	6.03	15.13	57.93	27.55
20	49	36	64.3	666031	183408	198342	61.29	6.05	15.18	57.79	27.30
20	59	38	74.3	666803	183710	198041	71.33	6.07	15.23	57.67	27.07
21	9	42	84.4	667120	184078	197886	81.39	6.07	15.27	57.62	26.87
21	19	44	94.4	668521	184444	197485	91.43	6.10	15.34	57.44	26.57
21	29	48	104.5	669206	184668	197066	101.49	6.12	15.39	57.31	26.33
21	39	50	114.5	670276	185055	196715	111.53	6.14	15.45	57.17	26.04
21	49	54	124.6	671378	185551	196967	121.59	6.14	15.47	57.15	25.94

$t_{correct.}$	Partial pressure (kPa)		Rate (mmol L^{-1} h^{-1})		d$[H_2O_2]$/dt	$\Sigma[H_2]$	$[H_2O_2]$	S_e	$\Sigma_2/[H_2O_2]$	$\Sigma_1/[H_2O_2]$
(min)	p_{H2}	p_{O2}	r_{H2}	r_{O2}	(mmol L^{-1} h^{-1})	(mmol L^{-1})	(mmol L^{-1})	(—)	(h)	(—)
0.00	14.09	35.05	74.48	53.51	32.53	0.00	0.00		0.000	0.000
11.06	14.09	35.12	74.40	53.05	31.69	13.72	5.92	0.43	0.092	2.318
21.09	14.09	35.18	74.33	52.63	30.93	26.16	11.16	0.43	0.177	2.345
31.16	14.09	35.25	74.27	52.22	30.17	38.62	16.28	0.42	0.263	2.372
41.19	14.09	35.32	74.18	51.76	29.35	51.04	21.26	0.42	0.349	2.401
51.23	14.09	35.37	74.13	51.38	28.63	63.44	26.11	0.41	0.436	2.430
61.29	14.12	35.43	73.94	50.91	27.89	75.86	30.85	0.41	0.524	2.459
71.33	14.13	35.49	73.79	50.48	27.18	88.21	35.45	0.40	0.612	2.488
81.39	14.13	35.55	73.72	50.11	26.49	100.58	39.95	0.40	0.701	2.517
91.43	14.16	35.62	73.50	49.56	25.62	112.89	44.31	0.39	0.791	2.548
101.49	14.18	35.68	73.33	49.10	24.87	125.21	48.55	0.39	0.883	2.579
111.53	14.20	35.75	73.14	48.57	23.99	137.46	52.63	0.38	0.975	2.612
121.59	14.20	35.78	73.12	48.37	23.62	149.73	56.63	0.38	1.068	2.644

H_2O_2 Synthesis Data Sheet

Entry No. 33 (Exp. Y50) Employed in: Fig. 4 Fig. 5 Fig. 9

Catalyst, Additives			Reaction conditions		Gas feed rate (sccm)				
Name	Conc.	(Unit)	T_0 (℃)	25.4		H_2	O_2	N_2	Sum
Pd-PVP	8.33	(mg/L)	T (℃)	30.4	Set	16.00	23.00	20.00	59.00
$Pt(NH_3)_4(NO_3)_2$	0.1667	(mg-Pt/L)	P_0 (hPa)	1006.0	Calibrated	16.00	21.25	20.30	57.55
H_2SO_4	0.01	(N)	P (hPa)	1013.2	Determination of final $[H_2O_2]$		Sample (g)	Absorbance (—)	$[H_2O_2]$ (mmol L^{-1})
NaBr	0.001	(N)	Agitation (rpm)	1202			0.505	0.845	56.44
Comment: Catalyst activation: H_2 gas 20 sccm at 303 K for 40 min.					Analysis of H_2O_2 formation selectivity and H_2O_2 destruction rate			S_f (—)	0.4358
								k_d[Cat] (h^{-1})	0.2014
								R^2	0.9999

GC calibration		GC count			Ratio of sensitivity (toward N_2)				Feed gas measurement	
Timing	No.	H_2	O_2	N_2	H_2		O_2			
Before reaction	1	1310468	191948	148703	0.0894	0.0893	0.811	0.811	T_a (℃)	25.3
	2	1312993	192392	149045	0.0895		0.811		P_0 (hPa)	1005.8
	3	1310698	191888	148481	0.0893		0.810		Flow	(cc/min)
After reaction	4	1307344	191172	148007	0.0892		0.810		H_2	18.19
	5	1307799	191302	148067	0.0892		0.810		O_2	24.16
	6	1307582	191284	148104	0.0893		0.810		N_2	23.08

Time				GC count				Outlet flow (sccm)		Conversion(%)	
H	M	S	min.	H_2	O_2	N_2	$t_{correct.}$ (min)	H_2	O_2	H_2	O_2
10	52	0	4.0	628502	115003	259728	0.00	6.72	14.60	57.99	31.32
11	2	2	14.0	735024	171908	203263	10.97	6.72	14.66	58.03	31.02
11	12	6	24.1	735393	177267	199019	21.04	6.71	14.72	58.06	30.75
11	22	8	34.1	733118	177974	198273	31.07	6.70	14.77	58.10	30.50
11	32	12	44.2	731560	178593	198009	41.14	6.70	14.84	58.13	30.16
11	42	14	54.2	729743	178832	197677	51.17	6.69	14.89	58.16	29.95
11	52	16	64.3	728623	179162	197236	61.20	6.70	14.95	58.13	29.67
12	2	20	74.3	727274	179850	197246	71.27	6.69	15.00	58.21	29.40
12	12	22	84.4	728069	180254	196972	81.30	6.70	15.06	58.11	29.14
12	22	26	94.4	724958	179842	195575	91.37	6.72	15.13	57.99	28.80
12	32	28	104.5	726573	180620	195609	101.40	6.73	15.19	57.91	28.51
12	42	32	114.5	728310	181203	195467	111.47	6.76	15.25	57.77	28.22
12	52	34	124.6	729936	181314	195087	121.50	6.78	15.29	57.60	28.04

$t_{correct.}$ (min)	Partial pressure (kPa)		Rate (mmol L^{-1} h^{-1})		$d[H_2O_2]/dt$ (mmol L^{-1} h^{-1})	$\Sigma[H_2]$ (mmol L^{-1})	$[H_2O_2]$ (mmol L^{-1})	S_e (—)	$\Sigma_2/[H_2O_2]$ (h)	$\Sigma_1/[H_2O_2]$ (—)
	p_{H2}	p_{O2}	r_{H2}	r_{O2}						
0.00	15.67	34.04	82.85	59.42	36.00	0.00	0.00		0.000	0.000
10.97	15.64	34.14	82.90	58.86	34.82	15.15	6.47	0.43	0.091	2.340
21.04	15.61	34.23	82.94	58.34	33.74	29.06	12.23	0.42	0.177	2.377
31.07	15.58	34.32	82.99	57.87	32.74	42.94	17.79	0.41	0.263	2.414
41.14	15.54	34.43	83.04	57.23	31.43	56.87	23.17	0.41	0.350	2.454
51.17	15.51	34.50	83.09	56.83	30.58	70.76	28.35	0.40	0.438	2.496
61.20	15.50	34.59	83.05	56.29	29.53	84.65	33.38	0.39	0.527	2.536
71.27	15.46	34.68	83.16	55.78	28.41	98.59	38.24	0.39	0.617	2.578
81.30	15.47	34.75	83.01	55.30	27.58	112.48	42.92	0.38	0.708	2.621
91.37	15.48	34.84	82.84	54.65	26.45	126.40	47.45	0.38	0.800	2.664
101.40	15.48	34.93	82.72	54.09	25.45	140.24	51.79	0.37	0.893	2.708
111.47	15.50	35.00	82.53	53.55	24.57	154.10	55.99	0.36	0.988	2.752
121.50	15.54	35.03	82.28	53.20	24.12	167.88	60.06	0.36	1.082	2.795

H_2O_2 Synthesis Data Sheet

Entry No. 34 (Exp. Y48) Employed in: Fig. 4 Fig. 5 Fig. 9

Catalyst, Additives			Reaction conditions		Gas feed rate (sccm)				
Name	Conc.	(Unit)	T_0 (℃)	25.2		H_2	O_2	N_2	Sum
Pd-PVP	8.33	(mg/L)	T (℃)	30.4	Set	16.00	24.00	20.00	60.00
$Pt(NH_3)_4(NO_3)_2$	0.25	(mg-Pt/L)	P_0 (hPa)	1000.2	Calibrated	16.11	22.25	20.38	58.74
H_2SO_4	0.01	(N)	P (hPa)	1007.5	Determination of final $[H_2O_2]$		Sample (g)	Absorbance (—)	$[H_2O_2]$ (mmol L^{-1})
NaBr	0.001	(N)	Agitation (rpm)	1200			0.693	1.142	56.59
Comment: Catalyst activation: H_2 gas 20 sccm at 303 K for 40 min.					Analysis of H_2O_2 formation selectivity and H_2O_2 destruction rate			S_f (—)	0.4237
								k_d[Cat] (h^{-1})	0.1503
								R^2	0.9998

GC calibration		GC count			Ratio of sensitivity (toward N_2)				Feed gas measurement	
Timing	No.	H_2	O_2	N_2	H_2		O_2			
Before reaction	1	1291266	197315	146642	0.0898	0.0895	0.811	0.811	T_a (℃)	24.8
	2	1291431	197102	146458	0.0896		0.811		P_0 (hPa)	1000.8
	3	1291907	197001	146326	0.0895		0.811		Flow	(cc/min)
After reaction	4	1287919	196049	145516	0.0893		0.810		H_2	18.36
	5	1288025	196096	145569	0.0893		0.810		O_2	25.36
	6	1288070	196097	145563	0.0893		0.810		N_2	23.23

Time				GC count			$t_{correct.}$	Outlet flow (sccm)		Conversion(%)	
H	M	S	min.	H_2	O_2	N_2	(min)	H_2	O_2	H_2	O_2
13	13	52	4.0	610786	120104	257384	0.00	6.37	15.33	60.44	31.12
13	23	54	14.0	694399	178966	201587	11.20	6.41	15.40	60.24	30.79
13	33	58	24.1	696246	184001	197123	21.27	6.43	15.47	60.05	30.48
13	44	0	34.1	696285	184663	196446	31.30	6.46	15.53	59.87	30.19
13	54	4	44.2	697500	185034	195857	41.37	6.49	15.61	59.68	29.84
14	4	6	54.2	698791	185268	195366	51.40	6.52	15.67	59.51	29.57
14	14	10	64.3	698946	185592	195003	61.47	6.54	15.73	59.42	29.32
14	24	12	74.3	699189	185769	194462	71.50	6.56	15.79	59.30	29.05
14	34	16	84.4	699965	186095	194049	81.57	6.58	15.85	59.16	28.78
14	44	18	94.4	699321	186157	193483	91.60	6.59	15.90	59.08	28.55
14	54	22	104.5	700561	186516	193136	101.67	6.61	15.96	58.94	28.28
15	4	24	114.5	702702	187051	192968	111.70	6.64	16.02	58.77	28.01
15	14	28	124.6	702702	187051	192968	121.77	6.64	16.02	58.77	28.01

$t_{correct.}$	Partial pressure (kPa)		Rate (mmol L^{-1} h^{-1})		$d[H_2O_2]/dt$	$\Sigma[H_2]$	$[H_2O_2]$	S_e	$\Sigma_2/[H_2O_2]$	$\Sigma_1/[H_2O_2]$
(min)	p_{H2}	p_{O2}	r_{H2}	r_{O2}	(mmol L^{-1} h^{-1})	(mmol L^{-1})	(mmol L^{-1})	(—)	(h)	(—)
0.00	14.61	35.14	86.93	61.83	36.74	0.00	0.00		0.000	0.000
11.20	14.65	35.22	86.64	61.16	35.69	16.21	6.76	0.42	0.093	2.396
21.27	14.68	35.30	86.37	60.55	34.73	30.72	12.67	0.41	0.178	2.425
31.30	14.72	35.37	86.12	59.98	33.84	45.14	18.40	0.41	0.264	2.453
41.37	14.75	35.46	85.84	59.28	32.72	59.57	23.99	0.40	0.351	2.483
51.40	14.78	35.52	85.59	58.75	31.92	73.90	29.39	0.40	0.438	2.514
61.47	14.79	35.59	85.47	58.25	31.03	88.25	34.67	0.39	0.526	2.545
71.50	14.81	35.66	85.28	57.72	30.16	102.53	39.79	0.39	0.615	2.577
81.57	14.83	35.73	85.09	57.17	29.25	116.82	44.77	0.38	0.705	2.609
91.60	14.84	35.79	84.98	56.71	28.45	131.04	49.59	0.38	0.796	2.642
101.67	14.86	35.85	84.77	56.18	27.60	145.28	54.30	0.37	0.887	2.676
111.70	14.89	35.92	84.53	55.65	26.77	159.43	58.84	0.37	0.979	2.710
121.77	14.89	35.92	84.53	55.65	26.77	173.62	63.33	0.36	1.072	2.741

H_2O_2 Synthesis Data Sheet

Entry No. 35 (Exp. Y47) Employed in: Fig. 4 Fig. 5 Fig. 9

Catalyst, Additives			Reaction conditions		Gas feed rate (sccm)				
Name	Conc.	(Unit)	T_0 (℃)	25.9		H_2	O_2	N_2	Sum
Pd-PVP	8.33	(mg/L)	T (℃)	30.5	Set	16.00	24.00	20.00	60.00
$Pt(NH_3)_4(NO_3)_2$	0.417	(mg-Pt/L)	P_0 (hPa)	1000.8	Calibrated	16.00	22.25	20.29	58.55
H_2SO_4	0.01	(N)	P (hPa)	1008.1	Determination of final $[H_2O_2]$		Sample (g)	Absorbance (—)	$[H_2O_2]$ (mmol L^{-1})
NaBr	0.001	(N)	Agitation (rpm)	1200			0.555	1.005	62.14
Comment: Catalyst activation: H_2 gas 20 sccm at 303 K for 40 min.					Analysis of H_2O_2 formation selectivity and H_2O_2 destruction rate			S_f (—)	0.4251
								k_d[Cat] (h^{-1})	0.1351
								R^2	0.9991

GC calibration		GC count			Ratio of sensitivity (toward N_2)				Feed gas measurement	
Timing	No.	H_2	O_2	N_2	H_2		O_2			
Before reaction	1	1284583	196159	145814	0.0895	0.0894	0.815	0.816	T_a (℃)	25.7
	2	1284395	196076	145784	0.0895		0.816		P_0 (hPa)	1001.8
	3	1284148	195923	145685	0.0895		0.816		Flow	(cc/min)
After reaction	4	1281780	195217	145141	0.0893		0.816		H_2	18.31
	5	1281804	195236	145128	0.0893		0.815		O_2	25.46
	6	1281216	195163	145091	0.0893		0.816		N_2	23.21

Time				GC count			$t_{correct.}$	Outlet flow (sccm)		Conversion(%)	
H	M	S	min.	H_2	O_2	N_2	(min)	H_2	O_2	H_2	O_2
18	4	26	4.0	606553	119746	255146	0.00	6.37	15.40	60.18	30.81
18	14	28	14.0	688543	177822	199842	11.17	6.40	15.46	59.99	30.51
18	24	32	24.1	690783	182773	195467	21.24	6.43	15.52	59.83	30.24
18	34	34	34.1	692882	183421	194718	31.27	6.46	15.59	59.66	29.97
18	44	38	44.2	693647	183589	194189	41.34	6.48	15.64	59.51	29.71
18	54	40	54.2	695252	183957	193789	51.37	6.51	15.71	59.33	29.43
19	4	42	64.3	693617	184160	193586	61.41	6.50	15.74	59.38	29.27
19	14	46	74.3	694457	184546	193307	71.47	6.52	15.80	59.28	29.02
19	24	48	84.4	693917	184726	192943	81.51	6.53	15.84	59.23	28.82
19	34	52	94.4	695286	185169	192614	91.57	6.55	15.91	59.08	28.53
19	44	54	104.5	695229	185410	192249	101.61	6.56	15.96	59.01	28.30
19	54	58	114.5	695920	185728	191951	111.67	6.58	16.01	58.90	28.07
20	5	0	124.6	697818	186164	191662	121.71	6.61	16.07	58.73	27.79

$t_{correct.}$	Partial pressure (kPa)		Rate (mmol L^{-1} h^{-1})		d$[H_2O_2]$/dt	$\Sigma[H_2]$	$[H_2O_2]$	S_e	$\Sigma_2/[H_2O_2]$	$\Sigma_1/[H_2O_2]$
(min)	p_{H2}	p_{O2}	r_{H2}	r_{O2}	(mmol L^{-1} h^{-1})	(mmol L^{-1})	(mmol L^{-1})	(—)	(h)	(—)
0.00	14.63	35.35	85.99	61.21	36.43	0.00	0.00		0.000	0.000
11.17	14.66	35.42	85.73	60.62	35.52	15.99	6.70	0.42	0.093	2.387
21.24	14.70	35.49	85.50	60.09	34.68	30.35	12.59	0.41	0.178	2.411
31.27	14.73	35.55	85.26	59.55	33.84	44.63	18.32	0.41	0.263	2.436
41.34	14.75	35.61	85.04	59.04	33.04	58.92	23.93	0.41	0.350	2.462
51.37	14.79	35.68	84.78	58.47	32.16	73.11	29.38	0.40	0.437	2.489
61.41	14.76	35.74	84.86	58.17	31.48	87.30	34.70	0.40	0.524	2.516
71.47	14.77	35.80	84.70	57.67	30.64	101.52	39.91	0.39	0.612	2.544
81.51	14.77	35.86	84.64	57.27	29.90	115.68	44.97	0.39	0.701	2.572
91.57	14.80	35.93	84.42	56.69	28.95	129.86	49.91	0.38	0.791	2.602
101.61	14.80	36.00	84.32	56.23	28.14	143.97	54.68	0.38	0.882	2.633
111.67	14.82	36.06	84.17	55.77	27.36	158.11	59.34	0.38	0.974	2.664
121.71	14.85	36.12	83.92	55.21	26.51	172.16	63.84	0.37	1.067	2.697

H_2O_2 Synthesis Data Sheet

Entry No. 36 (Exp. Y51) Employed in: Fig. 4 Fig. 5 Fig. 9

Catalyst, Additives			Reaction conditions		Gas feed rate (sccm)				
Name	Conc.	(Unit)	T_0 (℃)	25.5		H_2	O_2	N_2	Sum
Pd-PVP	8.33	(mg/L)	T (℃)	30.6	Set	18.50	25.00	20.00	63.50
$Pt(NH_3)_4(NO_3)_2$	0.417	(mg-Pt/L)	P_0 (hPa)	1006.0	Calibrated	18.57	23.18	20.25	62.00
H_2SO_4	0.01	(N)	P (hPa)	1013.6	Determination of final $[H_2O_2]$		Sample (g)	Absorbance (—)	$[H_2O_2]$ (mmol L^{-1})
NaBr	0.001	(N)	Agitation (rpm)	1200			0.585	1.109	65.10
Comment: Catalyst activation: H_2 gas 20 sccm at 303 K for 40 min.					Analysis of H_2O_2 formation selectivity and H_2O_2 destruction rate			S_f (—)	0.4055
								k_d[Cat] (h^{-1})	0.1852
								R^2	0.9998

GC calibration		GC count			Ratio of sensitivity (toward N_2)				Feed gas measurement	
Timing	No.	H_2	O_2	N_2	H_2		O_2			
Before reaction	1	1398155	193860	137926	0.0905	0.0905	0.814	0.814	T_a (℃)	25.7
	2	1398726	193833	137928	0.0904		0.815		P_0 (hPa)	1005.8
	3	1398317	193742	137892	0.0904		0.815		Flow	(cc/min)
After reaction	4	1399341	193962	137913	0.0904		0.814		H_2	21.16
	5	1399115	194040	138014	0.0905		0.814		O_2	26.41
	6	1399646	194180	138159	0.0905		0.815		N_2	23.07

Time				GC count			$t_{correct.}$	Outlet flow (sccm)		Conversion(%)	
H	M	S	min.	H_2	O_2	N_2	(min)	H_2	O_2	H_2	O_2
15	18	20	4.0	679666	119574	250037	0.00	7.29	15.26	60.75	34.17
15	28	22	14.0	770119	174846	196906	11.20	7.33	15.36	60.52	33.74
15	38	26	24.1	773580	179741	192604	21.26	7.37	15.45	60.32	33.35
15	48	28	34.1	775325	180678	191763	31.30	7.41	15.54	60.12	32.97
15	58	32	44.2	777645	181240	191165	41.36	7.45	15.63	59.88	32.55
16	8	34	54.2	778880	181745	190648	51.40	7.48	15.72	59.71	32.18
16	18	38	64.3	779732	182127	190230	61.46	7.51	15.79	59.57	31.89
16	28	40	74.3	781786	182778	189791	71.50	7.55	15.88	59.37	31.49
16	38	44	84.4	782674	183336	189624	81.56	7.56	15.94	59.29	31.22
16	48	46	94.4	782014	183083	188336	91.60	7.61	16.03	59.05	30.84
16	58	48	104.5	786747	184122	188309	101.63	7.65	16.12	58.79	30.44
17	8	52	114.5	788166	184571	187828	111.70	7.69	16.21	58.61	30.09
17	18	54	124.6	790402	185019	187442	121.73	7.72	16.28	58.41	29.78

$t_{correct.}$	Partial pressure (kPa)		Rate (mmol L^{-1} h^{-1})		$d[H_2O_2]/dt$	$\Sigma[H_2]$	$[H_2O_2]$	S_e	$\Sigma_2/[H_2O_2]$	$\Sigma_1/[H_2O_2]$
(min)	p_{H2}	p_{O2}	r_{H2}	r_{O2}	(mmol L^{-1} h^{-1})	(mmol L^{-1})	(mmol L^{-1})	(—)	(h)	(—)
0.00	16.54	34.61	100.74	70.73	40.72	0.00	0.00		0.000	0.000
11.20	16.58	34.73	100.36	69.84	39.31	18.77	7.47	0.40	0.093	2.513
21.26	16.61	34.83	100.02	69.03	38.04	35.57	13.96	0.39	0.179	2.549
31.30	16.65	34.93	99.70	68.24	36.77	52.27	20.21	0.39	0.265	2.586
41.36	16.70	35.03	99.29	67.37	35.45	68.97	26.27	0.38	0.352	2.625
51.40	16.72	35.13	99.01	66.60	34.19	85.55	32.09	0.38	0.440	2.666
61.46	16.74	35.21	98.78	66.00	33.21	102.14	37.75	0.37	0.530	2.706
71.50	16.78	35.31	98.45	65.16	31.88	118.63	43.19	0.36	0.620	2.747
81.56	16.78	35.39	98.32	64.61	30.90	135.14	48.45	0.36	0.711	2.789
91.60	16.83	35.47	97.91	63.83	29.75	151.54	53.52	0.35	0.803	2.831
101.63	16.88	35.57	97.49	63.00	28.50	167.88	58.39	0.35	0.896	2.875
111.70	16.91	35.65	97.19	62.28	27.36	184.21	63.08	0.34	0.991	2.920
121.73	16.95	35.72	96.86	61.63	26.40	200.44	67.58	0.34	1.087	2.966

H_2O_2 Synthesis Data Sheet

Entry No. 37 (Exp. G59) Employed in: Fig. 6

Catalyst, Additives			Reaction conditions		Gas feed rate (sccm)				
Name	Conc.	(Unit)	T_0 (℃)	20.5		H_2	O_2	N_2	Sum
Pd-PVP	8.33	(mg/L)	T (℃)	30.0	Set	5.00	20.00	20.00	45.00
$Pt(NH_3)_4(NO_3)_2$	0.0833	(mg-Pt/L)	P_0 (hPa)	1006.3	Calibrated	5.03	18.63	19.92	43.57
H_2SO_4	0.01	(N)	P (hPa)	1012.8	Determination of final $[H_2O_2]$		Sample (g)	Absorbance (—)	$[H_2O_2]$ (mmol L^{-1})
NaBr	0.001	(N)	Agitation (rpm)	1200			1.024	0.717	24.02
Comment: Catalyst activation: H_2 gas 20 sccm at 303 K for 40 min.					Analysis of H_2O_2 formation selectivity and H_2O_2 destruction rate			S_f (—)	0.5192
								k_d[Cat] (h^{-1})	0.0955
								R^2	0.9886

GC calibration		GC count			Ratio of sensitivity (toward N_2)				Feed gas measurement	
Timing	No.	H_2	O_2	N_2	H_2		O_2			
Before reaction	1	553641	215176	188804	0.0861	0.0861	0.821	0.821	T_a (℃)	20.0
	2	553189	215267	189080	0.0863		0.822		P_0 (hPa)	1006.2
	3	553785	215178	188804	0.0860		0.821		Flow	(cc/min)
After reaction	4	552668	214805	188480	0.0861		0.821		H_2	5.56
	5	553049	214757	188181	0.0859		0.820		O_2	20.61
	6	553316	214951	188572	0.0860		0.821		N_2	22.03

Time				GC count			$t_{correct.}$	Outlet flow (sccm)		Conversion(%)	
H	M	S	min.	H_2	O_2	N_2	(min)	H_2	O_2	H_2	O_2
14	17	0	4.0	212841	117416	286685	0.00	2.13	16.42	57.70	11.84
14	27	4	14.1	258033	199461	216437	10.82	2.13	16.44	57.59	11.74
14	37	6	24.1	259517	208235	208596	20.85	2.14	16.46	57.48	11.65
14	47	10	34.2	259476	209259	207550	30.92	2.14	16.48	57.37	11.54
14	57	12	44.2	260540	209863	207985	40.95	2.15	16.49	57.29	11.47
15	7	16	54.3	260514	209528	207366	51.02	2.15	16.52	57.16	11.35
15	17	18	64.3	261597	210165	207793	61.05	2.16	16.53	57.07	11.26
15	27	22	74.4	262008	210485	208212	71.12	2.16	16.53	57.09	11.31
15	37	24	84.4	262093	210128	207711	81.15	2.16	16.54	56.98	11.24
15	47	28	94.5	262416	210065	207214	91.22	2.17	16.57	56.82	11.06
15	57	30	104.5	262565	210045	207461	101.25	2.17	16.55	56.85	11.17
16	7	34	114.6	263026	210160	207496	111.32	2.17	16.56	56.78	11.14
16	17	36	124.6	263204	210150	207289	121.35	2.18	16.57	56.70	11.05

$t_{correct.}$	Partial pressure (kPa)		Rate (mmol L^{-1} h^{-1})		d$[H_2O_2]$/dt	$\Sigma[H_2]$	$[H_2O_2]$	S_e	$\Sigma_2/[H_2O_2]$	$\Sigma_1/[H_2O_2]$
(min)	p_{H2}	p_{O2}	r_{H2}	r_{O2}	(mmol L^{-1} h^{-1})	(mmol L^{-1})	(mmol L^{-1})	(—)	(h)	(—)
0.00	5.36	41.43	25.89	19.70	13.51	0.00	0.00		0.000	0.000
10.82	5.37	41.45	25.84	19.53	13.22	4.67	2.41	0.52	0.090	1.935
20.85	5.38	41.47	25.80	19.37	12.95	8.98	4.60	0.51	0.175	1.953
30.92	5.39	41.50	25.75	19.20	12.65	13.31	6.75	0.51	0.260	1.972
40.95	5.40	41.51	25.71	19.08	12.46	17.61	8.85	0.50	0.346	1.991
51.02	5.41	41.54	25.65	18.88	12.10	21.92	10.91	0.50	0.432	2.010
61.05	5.42	41.56	25.61	18.73	11.86	26.20	12.91	0.49	0.520	2.030
71.12	5.42	41.54	25.62	18.81	11.99	30.50	14.91	0.49	0.606	2.046
81.15	5.43	41.56	25.57	18.70	11.84	34.78	16.90	0.49	0.692	2.058
91.22	5.45	41.60	25.50	18.39	11.29	39.07	18.84	0.48	0.780	2.073
101.25	5.45	41.57	25.51	18.58	11.65	43.33	20.76	0.48	0.868	2.087
111.32	5.46	41.57	25.48	18.53	11.57	47.61	22.71	0.48	0.954	2.097
121.35	5.46	41.59	25.45	18.39	11.32	51.87	24.62	0.47	1.040	2.106

H_2O_2 Synthesis Data Sheet

Entry No. 38 (Exp. G61) Employed in: Fig. 6

Catalyst, Additives			Reaction conditions		Gas feed rate (sccm)				
Name	Conc.	(Unit)	T_0 (℃)	21.5		H_2	O_2	N_2	Sum
Pd-PVP	8.33	(mg/L)	T (℃)	30.0	Set	7.50	20.00	20.00	47.50
$Pt(NH_3)_4(NO_3)_2$	0.0833	(mg-Pt/L)	P_0 (hPa)	1015.0	Calibrated	7.50	18.61	20.02	46.13
H_2SO_4	0.01	(N)	P (hPa)	1021.4	Determination of final $[H_2O_2]$		Sample (g)	Absorbance (—)	$[H_2O_2]$ (mmol L^{-1})
NaBr	0.001	(N)	Agitation (rpm)	1200			1.255	1.323	36.24
Comment: Catalyst activation: H_2 gas 20 sccm at 303 K for 40 min.					Analysis of H_2O_2 formation selectivity and H_2O_2 destruction rate			S_f (—)	0.5074
								k_d[Cat] (h^{-1})	0.0694
								R^2	0.9988

GC calibration		GC count			Ratio of sensitivity (toward N_2)				Feed gas measurement	
Timing	No.	H_2	O_2	N_2	H_2		O_2			
Before reaction	1	772151	204266	178725	0.0867	0.0866	0.813	0.813	T_a (℃)	20.9
	2	772292	204345	178785	0.0867		0.813		P_0 (hPa)	1014.4
	3	772855	204394	178745	0.0866		0.813		Flow	(cc/min)
After reaction	4	772422	204179	178535	0.0865		0.813		H_2	8.26
	5	771816	203967	178280	0.0865		0.813		O_2	20.51
	6	771589	204003	178366	0.0866		0.813		N_2	22.06

Time				GC count			$t_{correct.}$	Outlet flow (sccm)		Conversion(%)	
H	M	S	min.	H_2	O_2	N_2	(min)	H_2	O_2	H_2	O_2
14	8	52	4.0	306829	111928	284374	0.00	3.07	15.27	59.10	17.94
14	18	54	14.0	369986	187512	218254	10.79	3.07	15.29	59.04	17.85
14	28	58	24.1	372128	196149	210585	20.86	3.08	15.31	58.98	17.76
14	39	0	34.1	371193	196743	209138	30.89	3.08	15.31	58.96	17.73
14	49	4	44.2	371966	196962	208660	40.96	3.09	15.37	58.78	17.45
14	59	6	54.2	371931	196989	208943	50.99	3.09	15.35	58.84	17.55
15	9	10	64.3	371931	197171	208904	61.06	3.09	15.36	58.83	17.46
15	19	12	74.3	371892	197171	208662	71.09	3.09	15.38	58.78	17.36
15	29	16	84.4	372546	197321	208635	81.16	3.10	15.40	58.71	17.29
15	39	18	94.4	372316	197396	208555	91.19	3.09	15.41	58.72	17.23
15	49	22	104.5	373060	197559	208546	101.26	3.10	15.42	58.63	17.15
15	59	24	114.5	372788	197628	208392	111.29	3.10	15.44	58.63	17.06
16	9	28	124.6	373112	198083	209054	121.36	3.09	15.42	58.73	17.14

$t_{correct.}$	Partial pressure (kPa)		Rate (mmol L^{-1} h^{-1})		$d[H_2O_2]/dt$	$\Sigma[H_2]$	$[H_2O_2]$	S_e	$\Sigma_2/[H_2O_2]$	$\Sigma_1/[H_2O_2]$
(min)	p_{H2}	p_{O2}	r_{H2}	r_{O2}	(mmol L^{-1} h^{-1})	(mmol L^{-1})	(mmol L^{-1})	(—)	(h)	(—)
0.00	7.82	38.98	39.56	29.82	20.08	0.00	0.00		0.000	0.000
10.79	7.83	39.00	39.51	29.66	19.81	7.11	3.59	0.50	0.090	1.982
20.86	7.84	39.02	39.47	29.51	19.55	13.73	6.89	0.50	0.174	1.994
30.89	7.84	39.03	39.46	29.47	19.47	20.33	10.15	0.50	0.259	2.003
40.96	7.86	39.10	39.34	29.00	18.66	26.94	13.35	0.50	0.344	2.018
50.99	7.86	39.07	39.38	29.17	18.96	33.53	16.49	0.49	0.430	2.033
61.06	7.85	39.10	39.37	29.01	18.66	40.13	19.65	0.49	0.515	2.042
71.09	7.86	39.12	39.34	28.86	18.37	46.71	22.74	0.49	0.601	2.054
81.16	7.87	39.14	39.29	28.73	18.17	53.31	25.81	0.48	0.687	2.065
91.19	7.87	39.16	39.30	28.63	17.96	59.88	28.83	0.48	0.774	2.077
101.26	7.88	39.17	39.24	28.51	17.78	66.47	31.83	0.48	0.861	2.088
111.29	7.87	39.20	39.24	28.36	17.48	73.03	34.78	0.48	0.948	2.100
121.36	7.86	39.18	39.31	28.48	17.65	79.62	37.72	0.47	1.035	2.111

H_2O_2 Synthesis Data Sheet

Entry No. 39 (Exp. G63) Employed in: Fig. 6

Catalyst, Additives			Reaction conditions		Gas feed rate (sccm)				
Name	Conc.	(Unit)	T_0 (℃)	18.4		H_2	O_2	N_2	Sum
Pd-PVP	8.33	(mg/L)	T (℃)	29.9	Set	10.00	20.00	20.00	50.00
$Pt(NH_3)_4(NO_3)_2$	0.0833	(mg-Pt/L)	P_0 (hPa)	1011.6	Calibrated	9.99	18.67	20.00	48.67
H_2SO_4	0.01	(N)	P (hPa)	1018.1	Determination of final $[H_2O_2]$		Sample (g)	Absorbance (—)	$[H_2O_2]$ (mmol L^{-1})
NaBr	0.001	(N)	Agitation (rpm)	1200					
							0.895	1.160	44.52
Comment: Catalyst activation: H_2 gas 20 sccm at 303 K for 40 min.					Analysis of H_2O_2 formation selectivity and H_2O_2 destruction rate			S_f (—)	0.4928
								k_d[Cat] (h^{-1})	0.1299
								R^2	0.9991

GC calibration		GC count			Ratio of sensitivity (toward N_2)				Feed gas measurement	
Timing	No.	H_2	O_2	N_2	H_2		O_2			
Before reaction	1	961696	196254	171920	0.0893	0.0882	0.818	0.814	T_a (℃)	18.1
	2	961283	195378	169985	0.0883		0.812		P_0 (hPa)	1012.4
	3	962882	195331	170220	0.0883		0.813		Flow	(cc/min)
After reaction	4	961412	194080	168995	0.0878		0.813		H_2	10.88
	5	960652	194002	169081	0.0879		0.814		O_2	20.34
	6	961406	194193	169342	0.0879		0.814		N_2	21.79

Time				GC count			$t_{correct.}$	Outlet flow (sccm)		Conversion(%)	
H	M	S	min.	H_2	O_2	N_2	(min)	H_2	O_2	H_2	O_2
10	27	58	4.0	407172	108181	280831	0.00	4.01	14.21	59.89	23.88
10	38	0	14.0	488613	176196	218485	11.03	4.00	14.24	59.91	23.73
10	48	4	24.1	481083	184228	212396	21.10	4.00	14.27	59.94	23.59
10	58	6	34.1	478091	185296	211003	31.13	4.00	14.30	59.96	23.43
11	8	10	44.2	477550	185431	210954	41.20	4.00	14.31	60.00	23.35
11	18	12	54.2	477126	185829	210835	51.23	3.99	14.35	60.01	23.15
11	28	14	64.3	476894	185863	210199	61.27	4.00	14.40	59.91	22.90
11	38	18	74.3	476533	186229	210357	71.33	4.00	14.41	59.97	22.80
11	48	20	84.4	476968	186342	209945	81.37	4.01	14.45	59.85	22.61
11	58	24	94.4	476422	186535	209721	91.43	4.01	14.48	59.86	22.44
12	8	26	104.5	476775	186679	209362	101.47	4.02	14.52	59.76	22.25
12	18	30	114.5	478014	186877	209082	111.53	4.04	14.55	59.60	22.06
12	28	32	124.6	478523	186960	208767	121.57	4.05	14.58	59.49	21.91

$t_{correct.}$	Partial pressure (kPa)		Rate (mmol L^{-1} h^{-1})		$d[H_2O_2]/dt$	$\Sigma[H_2]$	$[H_2O_2]$	S_e	$\Sigma_2/[H_2O_2]$	$\Sigma_1/[H_2O_2]$
(min)	p_{H2}	p_{O2}	r_{H2}	r_{O2}	(mmol L^{-1} h^{-1})	(mmol L^{-1})	(mmol L^{-1})	(—)	(h)	(—)
0.00	10.23	36.28	53.41	39.82	26.23	0.00	0.00		0.000	0.000
11.03	10.21	36.32	53.43	39.56	25.69	9.83	4.77	0.49	0.092	2.058
21.10	10.20	36.37	53.46	39.33	25.20	18.79	9.04	0.48	0.177	2.078
31.13	10.19	36.42	53.47	39.06	24.64	27.73	13.21	0.48	0.262	2.099
41.20	10.17	36.44	53.51	38.94	24.37	36.71	17.32	0.47	0.348	2.119
51.23	10.16	36.51	53.52	38.59	23.66	45.66	21.34	0.47	0.434	2.139
61.27	10.17	36.57	53.43	38.18	22.93	54.60	25.23	0.46	0.521	2.164
71.33	10.15	36.61	53.48	38.02	22.56	63.57	29.05	0.46	0.609	2.188
81.37	10.17	36.65	53.38	37.69	22.00	72.50	32.78	0.45	0.698	2.212
91.43	10.16	36.70	53.38	37.42	21.46	81.46	36.42	0.45	0.787	2.236
101.47	10.17	36.75	53.29	37.10	20.90	90.37	39.96	0.44	0.877	2.261
111.53	10.20	36.79	53.15	36.79	20.42	99.30	43.43	0.44	0.968	2.286
121.57	10.22	36.83	53.06	36.53	20.01	108.18	46.81	0.43	1.060	2.311

H_2O_2 Synthesis Data Sheet

Entry No. 40 (Exp. G10) Employed in: Fig. 6

Catalyst, Additives			Reaction conditions		Gas feed rate (sccm)				
Name	Conc.	(Unit)	T_0 (℃)	29.7		H_2	O_2	N_2	Sum
Pd-PVP	8.33	(mg/L)	T (℃)	30.0	Set	10.00	20.00	20.00	50.00
$Pt(NH_3)_4(NO_3)_2$	0.0833	(mg-Pt/L)	P_0 (hPa)	1005.2	Calibrated	9.94	18.39	20.22	48.55
H_2SO_4	0.01	(N)	P (hPa)	1011.7	Determination of final $[H_2O_2]$		Sample (g)	Absorbance (—)	$[H_2O_2]$ (mmol L^{-1})
NaBr	0.001	(N)	Agitation (rpm)	1200			0.791	1.263	54.85
Comment: Catalyst activation: H_2 gas 20 sccm at 303 K for 40 min.					Analysis of H_2O_2 formation selectivity and H_2O_2 destruction rate			S_f (—)	0.4865
								k_d[Cat] (h^{-1})	0.1410
								R^2	0.9995

GC calibration		GC count			Ratio of sensitivity (toward N_2)			Feed gas measurement	
Timing	No.	H_2	O_2	N_2	H_2		O_2		
Before reaction	1	944022	188149	170190	0.0887	0.0886	0.823	0.823	T_a (℃)	
	2	943908	188078	170094	0.0886		0.823		P_0 (hPa)	
	3	944098	188148	170212	0.0887		0.823		Flow	(cc/min)
After reaction	4	946475	188570	170494	0.0886		0.823		H_2	
	5	946274	188524	170399	0.0886		0.822		O_2	
	6	946515	188635	170510	0.0886		0.822		N_2	

Time				GC count			$t_{correct.}$	Outlet flow (sccm)		Conversion(%)	
H	M	S	min.	H_2	O_2	N_2	(min)	H_2	O_2	H_2	O_2
13	17	26	4.0	366362	103930	273188	0.00	4.12	14.06	58.55	23.55
13	27	28	14.0	428449	166734	216013	9.59	4.14	14.10	58.42	23.32
13	37	32	24.1	441968	173633	209294	19.66	4.15	14.15	58.29	23.08
13	47	34	34.1	477267	175374	205590	29.69	4.16	14.19	58.17	22.86
13	57	36	44.2	478352	175640	205109	39.72	4.18	14.24	57.98	22.57
14	7	40	54.2	479114	176002	205054	49.79	4.19	14.27	57.90	22.39
14	17	42	64.3	479245	176192	204922	59.82	4.19	14.30	57.86	22.25
14	27	46	74.3	479356	176411	204661	69.89	4.20	14.33	57.80	22.06
14	37	48	84.4	479853	176608	204494	79.92	4.20	14.36	57.72	21.91
14	47	52	94.4	480869	176843	204209	89.99	4.22	14.40	57.57	21.69
14	57	54	104.5	481919	177445	204584	100.02	4.22	14.42	57.55	21.57
15	7	58	114.5	482702	177666	204368	110.09	4.23	14.46	57.44	21.39
15	18	0	124.6	482846	177675	203828	120.12	4.24	14.50	57.32	21.18
15	28	4	134.6	483880	178122	204078	130.19	4.25	14.52	57.28	21.08
15	38	6	144.7	484144	178236	203664	140.22	4.26	14.55	57.17	20.86
15	48	10	154.7	484494	178313	203409	150.29	4.27	14.58	57.08	20.73

$t_{correct.}$	Partial pressure (kPa)		Rate (mmol L^{-1} h^{-1})		d$[H_2O_2]$/dt	Σ$[H_2]$	$[H_2O_2]$	S_e	$\Sigma_2/[H_2O_2]$	$\Sigma_1/[H_2O_2]$
(min)	p_{H2}	p_{O2}	r_{H2}	r_{O2}	(mmol L^{-1} h^{-1})	(mmol L^{-1})	(mmol L^{-1})	(—)	(h)	(—)
0.00	10.40	35.49	51.99	38.67	25.34	0.00	0.00		0.000	0.000
9.59	10.42	35.54	51.87	38.29	24.71	8.30	4.00	0.48	0.080	2.075
19.66	10.44	35.60	51.75	37.90	24.05	16.99	8.09	0.48	0.165	2.100
29.69	10.46	35.66	51.65	37.55	23.44	25.64	12.06	0.47	0.250	2.126
39.72	10.48	35.73	51.48	37.06	22.63	34.26	15.91	0.46	0.337	2.153
49.79	10.49	35.77	51.41	36.76	22.11	42.89	19.67	0.46	0.424	2.181
59.82	10.49	35.81	51.38	36.54	21.70	51.49	23.33	0.45	0.512	2.207
69.89	10.50	35.86	51.32	36.22	21.12	60.10	26.92	0.45	0.600	2.232
79.92	10.51	35.89	51.25	35.97	20.69	68.68	30.42	0.44	0.689	2.258
89.99	10.53	35.94	51.12	35.62	20.12	77.27	33.84	0.44	0.778	2.283
100.02	10.53	35.98	51.11	35.42	19.73	85.81	37.17	0.43	0.868	2.308
110.09	10.54	36.02	51.00	35.12	19.24	94.38	40.44	0.43	0.959	2.334
120.12	10.56	36.07	50.89	34.77	18.66	102.90	43.61	0.42	1.051	2.359
130.19	10.57	36.09	50.86	34.61	18.36	111.43	46.72	0.42	1.143	2.385
140.22	10.58	36.14	50.76	34.26	17.76	119.93	49.74	0.41	1.236	2.411
150.29	10.59	36.18	50.69	34.04	17.40	128.44	52.69	0.41	1.330	2.438

H_2O_2 Synthesis Data Sheet

Entry No. 41 (Exp. Y43) Employed in: Fig. 6

Catalyst, Additives			Reaction conditions		Gas feed rate (sccm)				
Name	Conc.	(Unit)	T_0 (℃)	25.4		H_2	O_2	N_2	Sum
Pd-PVP	8.33	(mg/L)	T (℃)	30.2	Set	14.60	20.00	20.00	54.60
$Pt(NH_3)_4(NO_3)_2$	0.0833	(mg-Pt/L)	P_0 (hPa)	1000.0	Calibrated	14.62	18.23	20.43	53.29
H_2SO_4	0.01	(N)	P (hPa)	1006.9	Determination of final $[H_2O_2]$		Sample (g)	Absorbance (—)	$[H_2O_2]$ (mmol L^{-1})
NaBr	0.001	(N)	Agitation (rpm)	1200			0.543	0.826	52.23
Comment: Catalyst activation: H_2 gas 20 sccm at 303 K for 40 min.					Analysis of H_2O_2 formation selectivity and H_2O_2 destruction rate			S_f (—)	0.6605
								k_d[Cat] (h^{-1})	0.5781
								R^2	0.9989

GC calibration		GC count			Ratio of sensitivity (toward N_2)				Feed gas measurement	
Timing	No.	H_2	O_2	N_2	H_2		O_2			
Before reaction	1	1286106	178221	159777	0.0889	0.0887	0.800	0.799	T_a (℃)	25.3
	2	1286479	178239	159732	0.0889		0.800		P_0 (hPa)	999.8
	3	1286237	178178	159678	0.0889		0.800		Flow	(cc/min)
After reaction	4	1287723	177788	159235	0.0885		0.799		H_2	16.73
	5	1287333	177923	159205	0.0885		0.799		O_2	20.86
	6	1287671	177903	159170	0.0885		0.799		N_2	23.37

Time				GC count			$t_{correct.}$	Outlet flow (sccm)		Conversion(%)	
H	M	S	min.	H_2	O_2	N_2	(min)	H_2	O_2	H_2	O_2
19	16	2	4.0	664422	103865	264291	0.00	7.89	12.65	46.07	30.65
19	26	6	14.1	859463	152041	205979	10.31	7.77	12.74	46.90	30.14
19	36	8	24.1	851717	157646	202536	20.34	7.65	12.83	47.70	29.64
19	46	12	34.2	839750	159774	202058	30.41	7.53	12.91	48.50	29.18
19	56	14	44.2	826356	161188	202106	40.44	7.41	13.03	49.34	28.57
20	6	18	54.3	814341	162184	202267	50.51	7.30	13.10	50.11	28.18
20	16	20	64.3	804822	163117	202429	60.54	7.20	13.16	50.73	27.83
20	26	24	74.4	796872	163694	202461	70.61	7.13	13.21	51.23	27.58
20	36	26	84.4	791934	164354	202504	80.64	7.09	13.26	51.54	27.31
20	46	30	94.5	787470	164868	202380	90.71	7.05	13.31	51.78	27.03
20	56	32	104.5	784738	165778	203294	100.74	7.00	13.32	52.17	26.96
21	6	36	114.6	779530	165523	202195	110.81	6.99	13.37	52.23	26.68
21	16	38	124.6	777330	166097	202477	120.84	6.96	13.40	52.43	26.53

$t_{correct.}$	Partial pressure (kPa)		Rate (mmol L^{-1} h^{-1})		$d[H_2O_2]/dt$	$\Sigma[H_2]$	$[H_2O_2]$	S_e	$\Sigma_2/[H_2O_2]$	$\Sigma_1/[H_2O_2]$
(min)	p_{H2}	p_{O2}	r_{H2}	r_{O2}	(mmol L^{-1} h^{-1})	(mmol L^{-1})	(mmol L^{-1})	(—)	(h)	(—)
0.00	18.57	29.78	60.15	49.90	39.64	0.00	0.00		0.000	0.000
10.31	18.30	30.02	61.24	49.06	36.89	10.43	6.58	0.63	0.086	1.586
20.34	18.03	30.25	62.29	48.25	34.22	20.76	12.52	0.60	0.173	1.658
30.41	17.77	30.47	63.33	47.50	31.67	31.30	18.05	0.58	0.262	1.734
40.44	17.49	30.74	64.42	46.51	28.60	41.98	23.09	0.55	0.354	1.818
50.51	17.24	30.94	65.43	45.88	26.33	52.87	27.70	0.52	0.449	1.909
60.54	17.03	31.11	66.25	45.31	24.36	63.88	31.94	0.50	0.545	2.000
70.61	16.87	31.24	66.89	44.91	22.93	75.05	35.90	0.48	0.643	2.090
80.64	16.76	31.36	67.30	44.46	21.62	86.27	39.63	0.46	0.742	2.177
90.71	16.67	31.46	67.62	44.02	20.41	97.59	43.15	0.44	0.843	2.261
100.74	16.56	31.53	68.12	43.90	19.68	108.94	46.50	0.43	0.943	2.343
110.81	16.52	31.62	68.20	43.44	18.67	120.37	49.72	0.41	1.044	2.421
120.84	16.45	31.68	68.46	43.19	17.92	131.80	52.78	0.40	1.146	2.497

H_2O_2 Synthesis Data Sheet

Entry No. 42 (Exp. G58) Employed in: Fig. 6

Catalyst, Additives			Reaction conditions		Gas feed rate (sccm)				
Name	Conc.	(Unit)	T_0 (℃)	18.4		H_2	O_2	N_2	Sum
Pd-PVP	8.33	(mg/L)	T (℃)	30.1	Set	15.00	25.00	15.00	55.00
$Pt(NH_3)_4(NO_3)_2$	0.0833	(mg-Pt/L)	P_0 (hPa)	1007.2	Calibrated	15.00	23.31	14.96	53.27
H_2SO_4	0.01	(N)	P (hPa)	1013.7	Determination of final $[H_2O_2]$		Sample (g)	Absorbance (—)	$[H_2O_2]$ (mmol L^{-1})
NaBr	0.001	(N)	Agitation (rpm)	1200			1.123	2.164	66.28
Comment: Catalyst activation: H_2 gas 20 sccm at 303 K for 40 min.					Analysis of H_2O_2 formation selectivity and H_2O_2 destruction rate			S_f (—)	0.7555
								k_d[Cat] (h^{-1})	0.5139
								R^2	0.9984

GC calibration		GC count			Ratio of sensitivity (toward N_2)				Feed gas measurement	
Timing	No.	H_2	O_2	N_2	H_2		O_2			
Before reaction	1	1283658	223122	117282	0.0916	0.0914	0.819	0.820	T_a (℃)	18.0
	2	1284250	222870	117331	0.0916		0.820		P_0 (hPa)	1008.6
	3	1284031	222633	117336	0.0916		0.821		Flow	(cc/min)
After reaction	4	1284433	221849	116867	0.0912		0.821		H_2	16.39
	5	1284350	221871	116835	0.0912		0.821		O_2	25.48
	6	1284427	222009	116806	0.0912		0.820		N_2	16.35

Time				GC count			$t_{correct.}$	Outlet flow (sccm)		Conversion(%)	
H	M	S	min.	H_2	O_2	N_2	(min)	H_2	O_2	H_2	O_2
10	13	14	4.0	624114	130722	242683	0.00	8.07	17.28	46.18	25.87
10	23	18	14.1	859212	206097	160645	9.81	7.95	17.35	46.98	25.58
10	33	20	24.1	863558	214637	152858	19.85	7.83	17.42	47.80	25.28
10	43	24	34.2	857037	216840	152303	29.91	7.69	17.47	48.70	25.05
10	53	26	44.2	845974	217873	151994	39.95	7.61	17.59	49.26	24.54
11	3	30	54.3	831698	219043	152632	50.01	7.45	17.61	50.32	24.45
11	13	32	64.3	818378	219985	152969	60.05	7.31	17.65	51.23	24.29
11	23	36	74.4	804945	220963	153389	70.11	7.17	17.68	52.16	24.16
11	33	38	84.4	736412	222577	157597	80.15	6.39	17.33	57.40	25.65
11	43	42	94.5	708231	223469	159534	90.21	6.07	17.19	59.53	26.26
11	53	44	104.5	714693	223972	159240	100.25	6.14	17.26	59.08	25.96
12	3	48	114.6	718019	224009	158060	110.31	6.21	17.39	58.59	25.39
12	13	50	124.6	721377	223909	157333	120.35	6.27	17.47	58.20	25.08

$t_{correct.}$	Partial pressure (kPa)		Rate (mmol L^{-1} h^{-1})		$d[H_2O_2]/dt$	$\Sigma[H_2]$	$[H_2O_2]$	S_e	$\Sigma_2/[H_2O_2]$	$\Sigma_1/[H_2O_2]$
(min)	p_{H2}	p_{O2}	r_{H2}	r_{O2}	(mmol L^{-1} h^{-1})	(mmol L^{-1})	(mmol L^{-1})	(—)	(h)	(—)
0.00	19.45	41.65	61.83	53.86	45.89	0.00	0.00		0.000	0.000
9.81	19.19	41.87	62.90	53.25	43.59	10.20	7.32	0.72	0.082	1.394
19.85	18.92	42.09	64.00	52.62	41.24	20.81	14.41	0.69	0.168	1.444
29.91	18.63	42.31	65.21	52.14	39.07	31.65	21.15	0.67	0.255	1.497
39.95	18.41	42.56	65.95	51.08	36.20	42.62	27.44	0.64	0.345	1.553
50.01	18.08	42.75	67.38	50.90	34.41	53.80	33.37	0.62	0.436	1.613
60.05	17.80	42.95	68.59	50.57	32.54	65.17	38.96	0.60	0.529	1.673
70.11	17.51	43.14	69.84	50.30	30.76	76.78	44.27	0.58	0.623	1.734
80.15	16.04	43.52	76.86	53.39	29.93	89.05	49.35	0.55	0.718	1.804
90.21	15.42	43.68	79.71	54.66	29.61	102.18	54.34	0.53	0.812	1.880
100.25	15.54	43.71	79.11	54.03	28.95	115.46	59.24	0.51	0.905	1.949
110.31	15.64	43.81	78.44	52.85	27.26	128.68	63.95	0.50	1.000	2.012
120.35	15.73	43.84	77.93	52.20	26.48	141.75	68.45	0.48	1.096	2.071

H_2O_2 Synthesis Data Sheet

Entry No. 43 (Exp. G60) Employed in: Fig. 6

Catalyst, Additives			Reaction conditions		Gas feed rate (sccm)				
Name	Conc.	(Unit)	T_0 (℃)	20.4		H_2	O_2	N_2	Sum
Pd-PVP	8.33	(mg/L)	T (℃)	30.1	Set	17.50	25.00	15.00	57.50
$Pt(NH_3)_4(NO_3)_2$	0.0833	(mg-Pt/L)	P_0 (hPa)	1015.0	Calibrated	17.39	23.21	15.03	55.63
H_2SO_4	0.01	(N)	P (hPa)	1022.0	Determination of final $[H_2O_2]$		Sample (g)	Absorbance (—)	$[H_2O_2]$ (mmol L^{-1})
NaBr	0.001	(N)	Agitation (rpm)	1200			0.749	1.538	70.61
Comment: Catalyst activation: H_2 gas 20 sccm at 303 K for 40 min.					Analysis of H_2O_2 formation selectivity and H_2O_2 destruction rate			S_f (—)	0.7435
								k_d[Cat] (h^{-1})	0.4680
								R^2	0.9992

GC calibration		GC count			Ratio of sensitivity (toward N_2)				Feed gas measurement	
Timing	No.	H_2	O_2	N_2	H_2		O_2			
Before reaction	1	1416465	213340	111884	0.0914	0.0913	0.810	0.811	T_a (℃)	20.7
	2	1417221	213137	111730	0.0912		0.810		P_0 (hPa)	1015.2
	3	1417106	213075	111965	0.0914		0.812		Flow	(cc/min)
After reaction	4	1421005	213123	111896	0.0911		0.811		H_2	19.13
	5	1421042	213100	111908	0.0911		0.811		O_2	25.53
	6	1423941	213628	112216	0.0912		0.811		N_2	16.53

Time				GC count			$t_{correct.}$	Outlet flow (sccm)		Conversion(%)	
H	M	S	min.	H_2	O_2	N_2	(min)	H_2	O_2	H_2	O_2
10	8	30	4.0	753809	126602	233213	0.00	9.59	16.42	44.84	29.27
10	18	32	14.0	1010252	193834	155323	10.04	9.49	16.53	45.45	28.79
10	28	36	24.1	1009498	201303	148793	20.11	9.38	16.64	46.05	28.31
10	38	38	34.1	1000470	203298	147958	30.14	9.27	16.74	46.68	27.87
10	48	42	44.2	988108	204647	147647	40.21	9.18	16.89	47.23	27.24
10	58	44	54.2	976834	205825	147819	50.24	9.06	16.97	47.89	26.91
11	8	48	64.3	968863	206791	147482	60.31	9.01	17.08	48.20	26.40
11	18	50	74.3	960329	207190	147097	70.34	8.95	17.16	48.52	26.06
11	28	54	84.4	960063	208284	147034	80.41	8.96	17.26	48.51	25.64
11	38	56	94.4	956493	209023	146876	90.44	8.93	17.34	48.65	25.30
11	48	58	104.5	955151	209954	146767	100.48	8.93	17.43	48.68	24.91
11	59	2	114.5	953214	210781	146747	110.54	8.91	17.50	48.78	24.60
12	9	4	124.6	948940	211427	146821	120.58	8.86	17.55	49.03	24.41

$t_{correct.}$	Partial pressure (kPa)		Rate (mmol L^{-1} h^{-1})		d[H_2O_2]/dt	Σ[H_2]	[H_2O_2]	S_e	$\Sigma_2/[H_2O_2]$	$\Sigma_1/[H_2O_2]$
(min)	p_{H2}	p_{O2}	r_{H2}	r_{O2}	(mmol L^{-1} h^{-1})	(mmol L^{-1})	(mmol L^{-1})	(—)	(h)	(—)
0.00	22.90	39.18	69.64	60.66	51.69	0.00	0.00		0.000	0.000
10.04	22.64	39.44	70.58	59.66	48.75	11.74	8.41	0.72	0.084	1.396
20.11	22.39	39.71	71.52	58.66	45.81	23.66	16.34	0.69	0.170	1.448
30.14	22.13	39.95	72.49	57.76	43.04	35.70	23.77	0.67	0.258	1.502
40.21	21.88	40.25	73.34	56.46	39.57	47.93	30.70	0.64	0.349	1.561
50.24	21.62	40.47	74.37	55.76	37.16	60.28	37.11	0.62	0.441	1.624
60.31	21.46	40.69	74.84	54.71	34.57	72.80	43.13	0.59	0.536	1.688
70.34	21.32	40.86	75.34	54.01	32.68	85.35	48.75	0.57	0.631	1.751
80.41	21.27	40.99	75.33	53.14	30.94	97.99	54.09	0.55	0.729	1.812
90.44	21.18	41.13	75.54	52.42	29.30	110.61	59.13	0.53	0.827	1.871
100.48	21.13	41.26	75.60	51.62	27.64	123.25	63.89	0.52	0.926	1.929
110.54	21.06	41.37	75.75	50.98	26.22	135.94	68.41	0.50	1.027	1.987
120.58	20.95	41.48	76.14	50.58	25.02	148.64	72.69	0.49	1.129	2.045

H_2O_2 Synthesis Data Sheet

Entry No. 44 (Exp. T334) Employed in: Fig. 6

Catalyst, Additives			Reaction conditions		Gas feed rate (sccm)				
Name	Conc.	(Unit)	T_0 (℃)	28.5		H_2	O_2	N_2	Sum
Pd-PVP	8.31	(mg/L)	T (℃)	29.9	Set	5.00	20.00	20.00	45.00
$Pt(NH_3)_4(NO_3)_2$	0.0833	(mg-Pt/L)	P_0 (hPa)	1001.0	Calibrated	5.05	18.08	20.41	43.54
H_2SO_4	0.01	(N)	P (hPa)	1007.3	Determination of final $[H_2O_2]$		Sample (g)	Absorbance (—)	$[H_2O_2]$ (mmol L^{-1})
NaBr	0.001	(N)	Agitation (rpm)	1201					
							1.621	1.149	24.43
Comment: Catalyst activation: H_2 gas 20 sccm at 303 K for 40 min.					Analysis of H_2O_2 formation selectivity and H_2O_2 destruction rate			S_f (—)	0.5142
								k_d[Cat] (h^{-1})	0.2213
								R^2	0.9663

GC calibration		GC count			Ratio of sensitivity (toward N_2)				Feed gas measurement	
Timing	No.	H_2	O_2	N_2	H_2		O_2			
Before reaction	1	872843	339074	305396	0.0866	0.0866	0.798	0.798	T_a (℃)	28.6
	2	881754	342473	308374	0.0865		0.798		P_0 (hPa)	1000.3
	3	882412	342666	308543	0.0865		0.798		Flow	(cc/min)
After reaction	4	890721	346315	311793	0.0866		0.798		H_2	5.88
	5	897575	348682	313797	0.0865		0.797		O_2	21.05
	6	898474	349390	314501	0.0866		0.797		N_2	23.76

Time				GC count			$t_{correct.}$	Outlet flow (sccm)		Conversion(%)	
H	M	S	min.	H_2	O_2	N_2	(min)	H_2	O_2	H_2	O_2
16	39	38	4.0	185046	108299	338725	0.00	1.81	15.61	64.08	13.65
16	49	40	14.0	244429	208927	253791	8.85	1.83	15.66	63.73	13.39
16	59	44	24.1	249507	226631	239753	18.91	1.85	15.71	63.33	13.08
17	9	46	34.1	251229	229480	236895	28.95	1.87	15.77	62.90	12.79
17	19	50	44.2	247982	225610	232018	39.01	1.89	15.83	62.61	12.45
17	29	52	54.2	253281	228054	233781	49.05	1.91	15.88	62.10	12.17
17	39	56	64.3	256153	230066	235766	59.11	1.92	15.88	61.99	12.14
17	49	58	74.3	257685	229723	235189	69.15	1.94	15.90	61.67	12.06
18	0	2	84.4	258421	229302	234592	79.21	1.95	15.91	61.46	12.00
18	10	4	94.4	259553	229893	235023	89.25	1.95	15.92	61.37	11.93
18	20	8	104.5	261229	230380	235396	99.31	1.96	15.93	61.18	11.89
18	30	10	114.5	261112	230241	235316	109.35	1.96	15.93	61.18	11.91
18	40	12	124.6	258073	227630	232367	119.38	1.96	15.95	61.15	11.80

$t_{correct.}$	Partial pressure (kPa)		Rate (mmol L^{-1} h^{-1})		$d[H_2O_2]/dt$	$\Sigma[H_2]$	$[H_2O_2]$	S_e	$\Sigma_2/[H_2O_2]$	$\Sigma_1/[H_2O_2]$
(min)	p_{H2}	p_{O2}	r_{H2}	r_{O2}	(mmol L^{-1} h^{-1})	(mmol L^{-1})	(mmol L^{-1})	(—)	(h)	(—)
0.00	4.63	39.82	28.89	22.04	15.18	0.00	0.00		0.000	0.000
8.85	4.66	39.87	28.74	21.61	14.48	4.25	2.19	0.51	0.074	1.943
18.91	4.71	39.93	28.56	21.12	13.67	9.06	4.55	0.50	0.160	1.991
28.95	4.75	39.99	28.36	20.64	12.92	13.81	6.77	0.49	0.247	2.040
39.01	4.78	40.06	28.23	20.10	11.98	18.56	8.86	0.48	0.337	2.095
49.05	4.84	40.11	28.00	19.65	11.30	23.26	10.81	0.46	0.428	2.153
59.11	4.85	40.11	27.95	19.60	11.25	27.96	12.70	0.45	0.520	2.202
69.15	4.88	40.12	27.81	19.47	11.13	32.62	14.57	0.45	0.609	2.239
79.21	4.91	40.12	27.71	19.37	11.02	37.28	16.43	0.44	0.699	2.269
89.25	4.92	40.14	27.67	19.26	10.85	41.91	18.26	0.44	0.788	2.296
99.31	4.94	40.14	27.59	19.19	10.79	46.54	20.07	0.43	0.877	2.319
109.35	4.94	40.13	27.59	19.22	10.86	51.16	21.88	0.43	0.964	2.338
119.38	4.94	40.16	27.57	19.05	10.53	55.77	23.67	0.42	1.052	2.356

H_2O_2 Synthesis Data Sheet

Entry No. 45 (Exp. T333) Employed in: Fig. 6

Catalyst, Additives			Reaction conditions		Gas feed rate (sccm)				
Name	Conc.	(Unit)	T_0 (℃)	28.7		H_2	O_2	N_2	Sum
Pd-PVP	8.31	(mg/L)	T (℃)	30.0	Set	11.50	20.00	20.00	51.50
$Pt(NH_3)_4(NO_3)_2$	0.0833	(mg-Pt/L)	P_0 (hPa)	1001.5	Calibrated	11.71	18.23	20.28	50.22
H_2SO_4	0.01	(N)	P (hPa)	1007.7	Determination of final $[H_2O_2]$		Sample (g)	Absorbance (—)	$[H_2O_2]$ (mmol L^{-1})
NaBr	0.001	(N)	Agitation (rpm)	1199					
							1.687	2.155	44.05
Comment: Catalyst activation: H_2 gas 20 sccm at 303 K for 40 min.					Analysis of H_2O_2 formation selectivity and H_2O_2 destruction rate			S_f (—)	0.4525
								k_d[Cat] (h^{-1})	0.1791
								R^2	0.9972

GC calibration		GC count			Ratio of sensitivity (toward N_2)				Feed gas measurement	
Timing	No.	H_2	O_2	N_2	H_2		O_2			
Before reaction	1	1562728	275599	247355	0.0914	0.0916	0.807	0.807	T_a (℃)	28.8
	2	1610231	284324	255235	0.0915		0.807		P_0 (hPa)	1002.7
	3	1629034	287581	258099	0.0914		0.807		Flow	(cc/min)
After reaction	4	1764017	312181	280234	0.0917		0.807		H_2	13.61
	5	1767572	312941	280962	0.0917		0.807		O_2	21.20
	6	1769011	313192	281166	0.0917		0.807		N_2	23.58

Time				GC count			$t_{correct.}$	Outlet flow (sccm)		Conversion(%)	
H	M	S	min.	H_2	O_2	N_2	(min)	H_2	O_2	H_2	O_2
12	15	42	4.0	412385	88729	304945	0.00	4.17	12.76	64.33	30.03
12	25	44	14.0	511148	168382	248382	8.76	4.19	12.82	64.18	29.71
12	35	48	24.1	536907	183664	238067	18.83	4.21	12.88	63.99	29.33
12	45	50	34.1	538981	186941	236404	28.86	4.23	12.94	63.83	29.02
12	55	54	44.2	543549	188782	236898	38.93	4.26	13.04	63.60	28.47
13	5	56	54.2	535403	185776	232466	48.96	4.28	13.08	63.46	28.26
13	16	0	64.3	550045	190663	237415	59.03	4.30	13.14	63.24	27.91
13	26	2	74.3	553825	191459	237614	69.06	4.33	13.19	63.02	27.67
13	36	4	84.4	556771	192767	238682	79.10	4.33	13.22	62.99	27.50
13	46	8	94.4	559209	193005	237969	89.16	4.36	13.27	62.72	27.20
13	56	10	104.5	556997	192754	237210	99.20	4.36	13.30	62.74	27.06
14	6	14	114.5	561936	193903	237698	109.26	4.39	13.35	62.49	26.77
14	16	16	124.6	564938	194606	237701	119.30	4.41	13.40	62.29	26.51

$t_{correct.}$	Partial pressure (kPa)		Rate (mmol L^{-1} h^{-1})		$d[H_2O_2]/dt$	$\Sigma[H_2]$	$[H_2O_2]$	S_e	$\Sigma_2/[H_2O_2]$	$\Sigma_1/[H_2O_2]$
(min)	p_{H2}	p_{O2}	r_{H2}	r_{O2}	(mmol L^{-1} h^{-1})	(mmol L^{-1})	(mmol L^{-1})	(—)	(h)	(—)
0.00	10.83	33.09	67.24	48.88	30.53	0.00	0.00		0.000	0.000
8.76	10.85	33.18	67.07	48.36	29.65	9.81	4.39	0.45	0.073	2.232
18.83	10.88	33.27	66.88	47.75	28.62	21.05	9.28	0.44	0.158	2.267
28.86	10.91	33.35	66.71	47.24	27.77	32.21	14.00	0.43	0.244	2.301
38.93	10.94	33.50	66.46	46.34	26.22	43.39	18.53	0.43	0.332	2.342
48.96	10.97	33.55	66.32	46.01	25.70	54.49	22.87	0.42	0.420	2.383
59.03	11.01	33.63	66.09	45.44	24.78	65.60	27.10	0.41	0.509	2.420
69.06	11.06	33.68	65.86	45.05	24.23	76.63	31.20	0.41	0.598	2.456
79.10	11.06	33.73	65.83	44.77	23.72	87.64	35.21	0.40	0.688	2.489
89.16	11.11	33.80	65.54	44.27	23.00	98.66	39.13	0.40	0.778	2.521
99.20	11.10	33.84	65.57	44.05	22.52	109.62	42.94	0.39	0.869	2.553
109.26	11.15	33.90	65.31	43.59	21.86	120.60	46.66	0.39	0.961	2.585
119.30	11.19	33.96	65.10	43.16	21.21	131.51	50.26	0.38	1.053	2.616

H_2O_2 Synthesis Data Sheet

Entry No. 46 (Exp. T335) Employed in: Fig. 6

Catalyst, Additives			Reaction conditions		Gas feed rate (sccm)				
Name	Conc.	(Unit)	T_0 (℃)	27.8		H_2	O_2	N_2	Sum
Pd-PVP	8.31	(mg/L)	T (℃)	29.9	Set	12.00	20.00	20.00	52.00
$Pt(NH_3)_4(NO_3)_2$	0.0833	(mg-Pt/L)	P_0 (hPa)	1004.2	Calibrated	12.14	17.92	20.38	50.43
H_2SO_4	0.01	(N)	P (hPa)	1010.4	Determination of final $[H_2O_2]$		Sample (g)	Absorbance (—)	$[H_2O_2]$ (mmol L^{-1})
NaBr	0.001	(N)	Agitation (rpm)	1200			1.709	2.301	46.41
Comment: Catalyst activation: H_2 gas 20 sccm at 303 K for 40 min.					Analysis of H_2O_2 formation selectivity and H_2O_2 destruction rate			S_f (—)	0.4261
								k_d[Cat] (h^{-1})	0.1635
								R^2	0.9978

GC calibration		GC count			Ratio of sensitivity (toward N_2)				Feed gas measurement	
Timing	No.	H_2	O_2	N_2	H_2		O_2			
Before reaction	1	1643781	278311	249202	0.0903	0.0905	0.788	0.788	T_a (℃)	28.4
	2	1678103	284392	254639	0.0904		0.788		P_0 (hPa)	1004.8
	3	1706744	289429	259238	0.0905		0.788		Flow	(cc/min)
After reaction	4	1821414	309628	277471	0.0907		0.788		H_2	14.05
	5	1823768	310038	277821	0.0907		0.788		O_2	20.75
	6	1818186	308985	276897	0.0907		0.788		N_2	23.59

Time				GC count			$t_{correct.}$	Outlet flow (sccm)		Conversion(%)	
H	M	S	min.	H_2	O_2	N_2	(min)	H_2	O_2	H_2	O_2
12	1	16	4.0	389361	86825	303351	0.00	4.27	12.31	64.78	31.31
12	11	18	14.0	498601	161137	244684	8.71	4.29	12.36	64.65	31.02
12	21	22	24.1	528440	178443	237135	18.77	4.31	12.42	64.50	30.68
12	31	24	34.1	549769	182415	234744	28.81	4.32	12.48	64.39	30.39
12	41	26	44.2	560348	185744	237383	38.84	4.36	12.56	64.11	29.91
12	51	30	54.2	561044	186386	237527	48.91	4.36	12.60	64.09	29.71
13	1	32	64.3	563945	187375	238010	58.94	4.37	12.64	63.98	29.48
13	11	36	74.3	563452	187521	237710	69.01	4.37	12.67	63.96	29.33
13	21	38	84.4	566373	188740	238717	79.04	4.38	12.69	63.93	29.17
13	31	42	94.4	561524	186615	235017	89.11	4.41	12.75	63.67	28.87
13	37	42	100.4	563336	188802	237652	95.11	4.37	12.75	63.96	28.83
13	47	46	110.5	569930	189118	236707	105.17	4.44	12.83	63.39	28.43
13	57	50	120.6	574044	190488	237702	115.24	4.46	12.87	63.28	28.21

$t_{correct.}$	Partial pressure (kPa)		Rate (mmol L^{-1} h^{-1})		$d[H_2O_2]/dt$	$\Sigma[H_2]$	$[H_2O_2]$	S_e	$\Sigma_2/[H_2O_2]$	$\Sigma_1/[H_2O_2]$
(min)	p_{H2}	p_{O2}	r_{H2}	r_{O2}	(mmol L^{-1} h^{-1})	(mmol L^{-1})	(mmol L^{-1})	(—)	(h)	(—)
0.00	11.19	32.24	70.19	50.10	30.01	0.00	0.00		0.000	0.000
8.71	11.21	32.32	70.05	49.64	29.22	10.18	4.30	0.42	0.073	2.368
18.77	11.24	32.41	69.89	49.09	28.30	21.92	9.12	0.42	0.158	2.402
28.81	11.25	32.49	69.77	48.63	27.48	33.59	13.79	0.41	0.243	2.437
38.84	11.30	32.61	69.47	47.86	26.25	45.24	18.28	0.40	0.330	2.475
48.91	11.30	32.67	69.44	47.54	25.63	56.89	22.63	0.40	0.418	2.514
58.94	11.32	32.73	69.32	47.17	25.02	68.49	26.87	0.39	0.506	2.549
69.01	11.31	32.77	69.31	46.94	24.57	80.12	31.03	0.39	0.595	2.582
79.04	11.32	32.81	69.27	46.68	24.10	91.71	35.10	0.38	0.684	2.613
89.11	11.37	32.88	68.99	46.20	23.40	103.31	39.08	0.38	0.773	2.643
95.11	11.29	32.92	69.30	46.14	22.97	110.22	41.40	0.38	0.827	2.662
105.17	11.42	32.99	68.69	45.49	22.30	121.80	45.20	0.37	0.918	2.695
115.24	11.44	33.04	68.57	45.15	21.72	133.31	48.89	0.37	1.010	2.727

H_2O_2 Synthesis Data Sheet

Entry No. 47 (Exp. T337) Employed in: Fig. 6

Catalyst, Additives			Reaction conditions		Gas feed rate (sccm)				
Name	Conc.	(Unit)	T_0 (℃)	29.4		H_2	O_2	N_2	Sum
Pd-PVP	8.31	(mg/L)	T (℃)	29.9	Set	11.50	20.00	20.00	51.50
$Pt(NH_3)_4(NO_3)_2$	0.0833	(mg-Pt/L)	P_0 (hPa)	1009.8	Calibrated	11.72	18.15	20.37	50.23
H_2SO_4	0.01	(N)	P (hPa)	1016.1	Determination of final $[H_2O_2]$		Sample (g)	Absorbance (—)	$[H_2O_2]$ (mmol L^{-1})
NaBr	0.001	(N)	Agitation (rpm)	1200					
							1.608	2.155	46.19
Comment: Catalyst activation: H_2 gas 20 sccm at 303 K for 40 min.					Analysis of H_2O_2 formation selectivity and H_2O_2 destruction rate			S_f (—)	0.4759
								k_d[Cat] (h^{-1})	0.2086
								R^2	0.9952

GC calibration		GC count			Ratio of sensitivity (toward N_2)				Feed gas measurement	
Timing	No.	H_2	O_2	N_2	H_2		O_2			
Before reaction	1	1642305	290013	259602	0.0909	0.0911	0.798	0.798	T_a (℃)	28.9
	2	1656860	292617	262272	0.0911		0.799		P_0 (hPa)	1010.7
	3	1701534	300764	269354	0.0911		0.798		Flow	(cc/min)
After reaction	4	1784037	315749	282850	0.0912		0.798		H_2	13.52
	5	1765872	312228	279688	0.0911		0.798		O_2	20.94
	6	1775987	314270	281791	0.0913		0.799		N_2	23.50

Time				GC count			$t_{correct.}$	Outlet flow (sccm)		Conversion(%)	
H	M	S	min.	H_2	O_2	N_2	(min)	H_2	O_2	H_2	O_2
12	3	40	4.0	416546	91162	310812	0.00	4.47	12.79	61.85	29.53
12	13	44	14.1	546709	168639	244777	8.80	4.47	12.84	61.87	29.23
12	23	46	24.1	561842	183280	234989	18.83	4.47	12.91	61.89	28.89
12	33	50	34.2	559653	185547	232751	28.90	4.46	12.96	61.92	28.58
12	43	52	44.2	561595	187388	233541	38.93	4.46	13.05	61.92	28.12
12	53	56	54.3	561208	188068	233643	49.00	4.46	13.09	61.96	27.89
13	3	58	64.3	561205	188727	233817	59.03	4.45	13.12	61.99	27.69
13	14	2	74.4	558370	188259	232725	69.10	4.45	13.15	62.00	27.53
13	24	4	84.4	555656	188065	232266	79.13	4.44	13.16	62.11	27.46
13	34	8	94.5	568634	192929	237333	89.20	4.45	13.22	62.05	27.17
13	44	10	104.5	567723	192972	236510	99.23	4.45	13.27	61.98	26.90
13	54	14	114.6	568379	193355	236955	109.30	4.45	13.27	62.01	26.90
14	4	16	124.6	564145	192196	235019	119.33	4.45	13.30	61.98	26.74

$t_{correct.}$	Partial pressure (kPa)		Rate (mmol L^{-1} h^{-1})		d$[H_2O_2]$/dt	$\Sigma[H_2]$	$[H_2O_2]$	S_e	$\Sigma_2/[H_2O_2]$	$\Sigma_1/[H_2O_2]$
(min)	p_{H2}	p_{O2}	r_{H2}	r_{O2}	(mmol L^{-1} h^{-1})	(mmol L^{-1})	(mmol L^{-1})	(—)	(h)	(—)
0.00	11.57	33.09	64.71	47.85	31.00	0.00	0.00		0.000	0.000
8.80	11.55	33.19	64.73	47.37	30.00	9.49	4.47	0.47	0.073	2.122
18.83	11.52	33.30	64.75	46.81	28.87	20.32	9.40	0.46	0.158	2.162
28.90	11.50	33.39	64.78	46.31	27.85	31.19	14.15	0.45	0.245	2.203
38.93	11.47	33.54	64.78	45.56	26.35	42.02	18.69	0.44	0.332	2.249
49.00	11.45	33.61	64.82	45.19	25.56	52.89	23.04	0.44	0.421	2.296
59.03	11.43	33.68	64.85	44.87	24.88	63.73	27.26	0.43	0.511	2.338
69.10	11.42	33.73	64.87	44.61	24.35	74.61	31.39	0.42	0.600	2.377
79.13	11.38	33.76	64.98	44.50	24.02	85.47	35.43	0.41	0.689	2.412
89.20	11.38	33.84	64.92	44.03	23.14	96.37	39.39	0.41	0.779	2.447
99.23	11.39	33.91	64.85	43.60	22.34	107.22	43.19	0.40	0.871	2.482
109.30	11.38	33.92	64.88	43.58	22.29	118.10	46.94	0.40	0.962	2.516
119.33	11.38	33.97	64.85	43.32	21.80	128.95	50.62	0.39	1.053	2.547

H_2O_2 Synthesis Data Sheet

Entry No. 48 (Exp. T344) Employed in: Fig. 6

Catalyst, Additives			Reaction conditions		Gas feed rate (sccm)				
Name	Conc.	(Unit)	T_0 (℃)	26.2		H_2	O_2	N_2	Sum
Pd-PVP	8.31	(mg/L)	T (℃)	30.1	Set	12.50	20.00	17.50	50.00
$Pt(NH_3)_4(NO_3)_2$	0.0833	(mg-Pt/L)	P_0 (hPa)	1008.8	Calibrated	12.79	18.34	17.59	48.72
H_2SO_4	0.01	(N)	P (hPa)	1014.4	Determination of final $[H_2O_2]$		Sample (g)	Absorbance (—)	$[H_2O_2]$ (mmol L^{-1})
NaBr	0.001	(N)	Agitation (rpm)	1201					
							0.615	1.009	56.55
Comment: Catalyst activation: H_2 gas 20 sccm at 303 K for 40 min.					Analysis of H_2O_2 formation selectivity and H_2O_2 destruction rate			S_f (—)	0.4603
								k_d[Cat] (h^{-1})	0.1905
								R^2	0.9952

GC calibration		GC count			Ratio of sensitivity (toward N_2)				Feed gas measurement	
Timing	No.	H_2	O_2	N_2	H_2		O_2			
Before reaction	1	1976983	324001	253515	0.0932	0.0932	0.816	0.815	T_a (℃)	26.4
	2	1968563	322537	252302	0.0932		0.815		P_0 (hPa)	1008.2
	3	1982471	324948	254238	0.0932		0.816		Flow	(cc/min)
After reaction	4	2032745	333346	260757	0.0933		0.815		H_2	14.59
	5	2030091	333055	260547	0.0933		0.815		O_2	20.92
	6	2043251	335302	262256	0.0933		0.815		N_2	20.07

Time				GC count			$t_{correct.}$	Outlet flow (sccm)		Conversion(%)	
H	M	S	min.	H_2	O_2	N_2	(min)	H_2	O_2	H_2	O_2
16	11	56	4.0	473758	96064	328466	0.00	4.36	12.17	65.92	33.63
16	22	0	14.1	616422	183746	251104	8.27	4.36	12.23	65.89	33.32
16	32	2	24.1	623295	199784	238796	18.30	4.36	12.30	65.87	32.95
16	42	6	34.2	631517	204342	237218	28.37	4.37	12.36	65.85	32.61
16	52	8	44.2	629781	204992	236200	38.40	4.37	12.45	65.80	32.11
17	2	12	54.3	629849	205784	236232	48.47	4.37	12.50	65.80	31.85
17	12	14	64.3	628114	205902	235660	58.50	4.37	12.53	65.81	31.65
17	22	18	74.4	630171	206893	236047	68.57	4.38	12.57	65.76	31.43
17	32	20	84.4	619946	203917	232213	78.60	4.38	12.60	65.76	31.30
17	42	24	94.5	627909	208345	236671	88.67	4.35	12.63	65.97	31.13
17	52	26	104.5	630227	208521	235965	98.70	4.38	12.68	65.74	30.87
18	2	30	114.6	629390	209131	236241	108.77	4.37	12.70	65.83	30.75
18	12	32	124.6	629643	209740	236418	118.80	4.37	12.73	65.84	30.60

$t_{correct.}$	Partial pressure (kPa)		Rate (mmol L^{-1} h^{-1})		$d[H_2O_2]/dt$	$\Sigma[H_2]$	$[H_2O_2]$	S_e	$\Sigma_2/[H_2O_2]$	$\Sigma_1/[H_2O_2]$
(min)	p_{H2}	p_{O2}	r_{H2}	r_{O2}	(mmol L^{-1} h^{-1})	(mmol L^{-1})	(mmol L^{-1})	(—)	(h)	(—)
0.00	12.42	34.67	75.27	55.06	34.86	0.00	0.00		0.000	0.000
8.27	12.40	34.77	75.24	54.56	33.87	10.37	4.74	0.46	0.069	2.190
18.30	12.39	34.89	75.21	53.94	32.67	22.95	10.30	0.45	0.154	2.228
28.37	12.37	35.00	75.19	53.40	31.60	35.57	15.69	0.44	0.240	2.267
38.40	12.35	35.16	75.13	52.57	30.00	48.14	20.84	0.43	0.327	2.310
48.47	12.34	35.25	75.14	52.15	29.17	60.74	25.81	0.42	0.416	2.354
58.50	12.32	35.32	75.15	51.82	28.49	73.31	30.63	0.42	0.504	2.394
68.57	12.32	35.38	75.08	51.46	27.84	85.91	35.35	0.41	0.594	2.430
78.60	12.31	35.42	75.08	51.25	27.42	98.47	39.97	0.41	0.683	2.463
88.67	12.24	35.51	75.33	50.97	26.62	111.09	44.51	0.40	0.772	2.496
98.70	12.29	35.56	75.07	50.54	26.01	123.66	48.91	0.40	0.862	2.529
108.77	12.26	35.61	75.17	50.34	25.52	136.26	53.23	0.39	0.953	2.560
118.80	12.24	35.66	75.18	50.10	25.02	148.83	57.46	0.39	1.044	2.590

H_2O_2 Synthesis Data Sheet

Entry No. 49 (Exp. T345) Employed in: Fig. 6

Catalyst, Additives			Reaction conditions		Gas feed rate (sccm)				
Name	Conc.	(Unit)	T_0 (℃)	27.4		H_2	O_2	N_2	Sum
Pd-PVP	8.31	(mg/L)	T (℃)	30.4	Set	13.00	20.00	17.00	50.00
$Pt(NH_3)_4(NO_3)_2$	0.0833	(mg-Pt/L)	P_0 (hPa)	1006.3	Calibrated	13.14	18.27	16.97	48.38
H_2SO_4	0.01	(N)	P (hPa)	1011.8	Determination of final $[H_2O_2]$		Sample (g)	Absorbance (—)	$[H_2O_2]$ (mmol L^{-1})
NaBr	0.001	(N)	Agitation (rpm)	1201					
							0.675	1.116	56.99
Comment: Catalyst activation: H_2 gas 20 sccm at 303 K for 40 min.					Analysis of H_2O_2 formation selectivity and H_2O_2 destruction rate			S_f (—)	0.4995
								k_d[Cat] (h^{-1})	0.2942
								R^2	0.9844

GC calibration		GC count			Ratio of sensitivity (toward N_2)				Feed gas measurement	
Timing	No.	H_2	O_2	N_2	H_2		O_2			
Before reaction	1	2129216	337899	257181	0.0936	0.0936	0.819	0.819	T_a (℃)	27.0
	2	2150274	341329	259796	0.0936		0.819		P_0 (hPa)	1007.2
	3	2169294	344310	262222	0.0936		0.820		Flow	(cc/min)
After reaction	4	2243107	356453	271196	0.0937		0.819		H_2	15.06
	5	2236406	355395	270494	0.0937		0.819		O_2	20.93
	6	2233321	354973	270187	0.0937		0.819		N_2	19.44

Time				GC count			$t_{correct.}$	Outlet flow (sccm)		Conversion(%)	
H	M	S	min.	H_2	O_2	N_2	(min)	H_2	O_2	H_2	O_2
15	42	54	4.0	530777	99343	340481	0.00	4.40	11.68	66.52	36.09
15	52	56	14.0	772016	187732	249895	8.10	4.41	11.78	66.48	35.53
16	2	58	24.1	780305	203612	237386	18.13	4.41	11.91	66.42	34.82
16	13	2	34.1	675251	209335	242167	28.20	4.43	12.02	66.29	34.20
16	23	4	44.2	668366	211286	240806	38.23	4.41	12.20	66.45	33.22
16	33	8	54.2	670080	211546	239499	48.30	4.45	12.28	66.18	32.77
16	43	10	64.3	669020	211779	238924	58.33	4.45	12.32	66.15	32.53
16	53	14	74.3	669787	212251	238904	68.40	4.45	12.35	66.11	32.38
17	3	16	84.4	669417	212656	238488	78.43	4.46	12.40	66.07	32.13
17	13	20	94.4	671063	213346	238602	88.50	4.47	12.43	66.00	31.94
17	23	22	104.5	670574	213580	238245	98.53	4.47	12.46	65.97	31.76
17	33	26	114.5	671523	214367	238548	108.60	4.47	12.49	65.97	31.60
17	43	28	124.6	670490	214344	237722	118.63	4.48	12.54	65.90	31.37

$t_{correct.}$	Partial pressure (kPa)		Rate (mmol L^{-1} h^{-1})		$d[H_2O_2]/dt$	$\Sigma[H_2]$	$[H_2O_2]$	S_e	$\Sigma_2/[H_2O_2]$	$\Sigma_1/[H_2O_2]$
(min)	p_{H2}	p_{O2}	r_{H2}	r_{O2}	(mmol L^{-1} h^{-1})	(mmol L^{-1})	(mmol L^{-1})	(—)	(h)	(—)
0.00	12.91	34.25	78.07	58.86	39.66	0.00	0.00		0.000	0.000
8.10	12.88	34.44	78.01	57.94	37.87	10.53	5.23	0.50	0.067	2.013
18.13	12.85	34.67	77.95	56.80	35.65	23.57	11.38	0.48	0.153	2.072
28.20	12.85	34.87	77.80	55.79	33.78	36.64	17.20	0.47	0.241	2.130
38.23	12.73	35.22	77.98	54.18	30.37	49.66	22.57	0.45	0.331	2.201
48.30	12.79	35.33	77.67	53.45	29.23	62.72	27.56	0.44	0.423	2.275
58.33	12.78	35.41	77.63	53.06	28.49	75.71	32.39	0.43	0.515	2.337
68.40	12.79	35.46	77.58	52.81	28.03	88.73	37.13	0.42	0.606	2.389
78.43	12.78	35.53	77.54	52.40	27.27	101.70	41.76	0.41	0.697	2.436
88.50	12.79	35.59	77.46	52.10	26.74	114.70	46.29	0.40	0.788	2.478
98.53	12.79	35.64	77.43	51.81	26.19	127.65	50.71	0.40	0.880	2.517
108.60	12.78	35.70	77.42	51.54	25.66	140.64	55.06	0.39	0.971	2.554
118.63	12.78	35.76	77.34	51.17	24.99	153.58	59.30	0.39	1.063	2.590

H_2O_2 Synthesis Data Sheet

Entry No. 50 (Exp. T339) Employed in: Fig. 6

Catalyst, Additives			Reaction conditions		Gas feed rate (sccm)				
Name	Conc.	(Unit)	T_0 (℃)	26.6		H_2	O_2	N_2	Sum
Pd-PVP	8.31	(mg/L)	T (℃)	30.1	Set	17.50	25.00	15.00	57.50
$Pt(NH_3)_4(NO_3)_2$	0.0833	(mg-Pt/L)	P_0 (hPa)	1007.0	Calibrated	17.66	22.90	15.13	55.69
H_2SO_4	0.01	(N)	P (hPa)	1013.4	Determination of final $[H_2O_2]$		Sample (g)	Absorbance (—)	$[H_2O_2]$ (mmol L^{-1})
NaBr	0.001	(N)	Agitation (rpm)	1200			0.945	2.097	76.51
Comment: Catalyst activation: H_2 gas 20 sccm at 303 K for 40 min.					Analysis of H_2O_2 formation selectivity and H_2O_2 destruction rate			S_f (—)	0.7253
								k_d[Cat] (h^{-1})	0.5998
								R^2	0.9985

GC calibration		GC count			Ratio of sensitivity (toward N_2)				Feed gas measurement	
Timing	No.	H_2	O_2	N_2	H_2		O_2			
Before reaction	1	2343829	351362	189669	0.0944	0.0944	0.817	0.816	T_a (℃)	26.3
	2	2353212	352581	190176	0.0943		0.816		P_0 (hPa)	1007.4
	3	2360035	353571	190716	0.0943		0.816		Flow	(cc/min)
After reaction	4	2403767	360302	194451	0.0944		0.817		H_2	20.15
	5	2425923	363831	196140	0.0943		0.816		O_2	26.13
	6	2407572	360993	194782	0.0944		0.816		N_2	17.27

Time				GC count			$t_{correct.}$	Outlet flow (sccm)		Conversion(%)	
H	M	S	min.	H_2	O_2	N_2	(min)	H_2	O_2	H_2	O_2
16	12	50	4.0	667526	106474	278606	0.00	8.33	14.90	52.82	34.92
16	22	54	14.1	943708	192795	186853	8.87	8.18	15.01	53.66	34.43
16	32	56	24.1	944564	205673	172663	18.90	8.01	15.14	54.61	33.88
16	43	0	34.2	933038	209719	169875	28.97	7.84	15.25	55.58	33.40
16	53	2	44.2	936861	217233	174045	39.00	7.69	15.42	56.47	32.66
17	3	6	54.3	898892	214509	170947	49.07	7.51	15.50	57.48	32.30
17	13	8	64.3	881818	217421	172862	59.10	7.28	15.54	58.75	32.14
17	23	12	74.4	774595	219503	180359	69.17	6.13	15.03	65.27	34.34
17	33	14	84.4	784514	223412	182395	79.20	6.14	15.13	65.22	33.92
17	43	18	94.5	782084	221277	179090	89.27	6.24	15.26	64.69	33.34
17	53	20	104.5	793831	225358	181421	99.30	6.25	15.35	64.62	32.99
18	3	24	114.6	795234	224385	179468	109.37	6.33	15.45	64.17	32.55
18	13	26	124.6	805216	227929	181349	119.40	6.34	15.53	64.09	32.19

$t_{correct.}$	Partial pressure (kPa)		Rate (mmol L^{-1} h^{-1})		$d[H_2O_2]/dt$	$\Sigma[H_2]$	$[H_2O_2]$	S_e	$\Sigma_2/[H_2O_2]$	$\Sigma_1/[H_2O_2]$
(min)	p_{H2}	p_{O2}	r_{H2}	r_{O2}	(mmol L^{-1} h^{-1})	(mmol L^{-1})	(mmol L^{-1})	(—)	(h)	(—)
0.00	21.08	37.71	83.27	71.39	59.51	0.00	0.00		0.000	0.000
8.87	20.73	38.03	84.60	70.40	56.20	12.41	8.55	0.69	0.074	1.451
18.90	20.32	38.39	86.10	69.28	52.45	26.68	17.64	0.66	0.160	1.513
28.97	19.92	38.74	87.63	68.28	48.93	41.25	26.14	0.63	0.248	1.578
39.00	19.52	39.15	89.03	66.78	44.53	56.02	33.95	0.61	0.339	1.650
49.07	19.11	39.46	90.62	66.04	41.47	71.09	41.17	0.58	0.433	1.727
59.10	18.63	39.75	92.62	65.72	38.82	86.41	47.88	0.55	0.528	1.805
69.17	16.40	40.20	102.90	70.21	37.52	102.82	54.28	0.53	0.623	1.894
79.20	16.37	40.34	102.82	69.35	35.87	120.02	60.42	0.50	0.719	1.986
89.27	16.52	40.44	101.98	68.17	34.35	137.20	66.31	0.48	0.815	2.069
99.30	16.51	40.56	101.87	67.44	33.00	154.24	71.94	0.47	0.912	2.144
109.37	16.64	40.62	101.16	66.54	31.92	171.27	77.39	0.45	1.010	2.213
119.40	16.63	40.73	101.05	65.82	30.59	188.18	82.62	0.44	1.108	2.278

H_2O_2 Synthesis Data Sheet

Entry No. 51 (Exp. T017) Employed in: Fig. 9

Catalyst, Additives			Reaction conditions		Gas feed rate (sccm)				
Name	Conc.	(Unit)	T_0 (℃)	27.3		H_2	O_2	N_2	Sum
Pt-PVP	1.04	(mg/L)	T (℃)	30.2	Set	2.50	20.00	27.50	50.00
			P_0 (hPa)	1009.3	Calibrated	2.65	18.73	27.25	48.63
			P (hPa)	1017.5	Determination of final $[H_2O_2]$		Sample (g)	Absorbance (—)	$[H_2O_2]$ (mmol L^{-1})
			Agitation (rpm)	1200					
							1.892	0.010	0.18
Comment: Catalyst activation: H_2 gas 20 sccm at 303 K for 40 min.					Analysis of H_2O_2 formation selectivity and H_2O_2 destruction rate			S_f (—)	0.1199
								k_d[Cat] (h^{-1})	2.2006
								R^2	0.9784

GC calibration		GC count			Ratio of sensitivity (toward N_2)				Feed gas measurement	
Timing	No.	H_2	O_2	N_2	H_2		O_2			
Before reaction	1	262977	202208	242952	0.0898	0.0885	0.826	0.825	T_a (℃)	27.7
	2	264515	201892	242605	0.0892		0.826		P_0 (hPa)	1009.6
	3	265064	201896	242347	0.0889		0.825		Flow	(cc/min)
After reaction	4	266887	200464	240810	0.0877		0.826		H_2	3.04
	5	267097	200670	240940	0.0877		0.825		O_2	21.49
	6	266746	200620	240976	0.0878		0.825		N_2	31.27

Time				GC count			$t_{correct.}$	Outlet flow (sccm)		Conversion(%)	
H	M	S	min.	H_2	O_2	N_2	(min)	H_2	O_2	H_2	O_2
15	43	50	4.0	186115	121195	298933	0.00	1.95	18.34	26.35	2.07
15	53	54	14.1	188444	189657	242636	9.88	1.97	18.36	25.49	1.96
16	3	56	24.1	195414	194159	238191	19.92	2.00	18.38	24.62	1.85
16	13	58	34.1	198478	193926	237089	29.95	2.02	18.40	23.78	1.76
16	24	2	44.2	201164	194357	237256	40.02	2.05	18.43	22.80	1.61
16	34	4	54.2	202926	194242	236941	50.05	2.07	18.44	22.02	1.53
16	44	8	64.3	204133	194095	236714	60.12	2.08	18.45	21.48	1.52
16	54	10	74.3	205390	194019	236552	70.15	2.09	18.45	20.94	1.49
17	4	14	84.4	206224	193771	236158	80.22	2.11	18.46	20.49	1.45
17	14	16	94.4	207345	193646	236085	90.25	2.12	18.45	20.03	1.48
17	24	20	104.5	208482	193821	236302	100.32	2.13	18.45	19.67	1.48
17	34	22	114.5	209449	194200	236506	110.35	2.14	18.47	19.37	1.38
17	44	26	124.6	210277	194273	236563	120.42	2.14	18.48	19.07	1.36

$t_{correct.}$	Partial pressure (kPa)		Rate (mmol L^{-1} h^{-1})		$d[H_2O_2]/dt$	$\Sigma[H_2]$	$[H_2O_2]$	S_e	$\Sigma_2/[H_2O_2]$	$\Sigma_1/[H_2O_2]$
(min)	p_{H2}	p_{O2}	r_{H2}	r_{O2}	(mmol L^{-1} h^{-1})	(mmol L^{-1})	(mmol L^{-1})	(—)	(h)	(—)
0.00	4.00	37.61	6.23	3.47	0.70	0.00	0.00		0.000	0.000
9.88	4.04	37.62	6.03	3.28	0.54	1.01	0.10	0.10	0.082	9.922
19.92	4.09	37.63	5.82	3.10	0.38	2.00	0.18	0.09	0.178	11.220
29.95	4.13	37.64	5.62	2.94	0.25	2.96	0.23	0.08	0.286	12.820
40.02	4.18	37.65	5.39	2.69	-0.02	3.88	0.25	0.06	0.425	15.516
50.05	4.22	37.65	5.21	2.57	-0.08	4.77	0.24	0.05	0.609	19.671
60.12	4.25	37.65	5.08	2.53	-0.01	5.63	0.23	0.04	0.799	23.979
70.15	4.27	37.64	4.95	2.49	0.02	6.47	0.24	0.04	0.965	27.535
80.22	4.30	37.64	4.85	2.42	0.00	7.29	0.24	0.03	1.129	30.902
90.25	4.32	37.62	4.74	2.48	0.21	8.10	0.25	0.03	1.212	31.922
100.32	4.34	37.62	4.65	2.48	0.31	8.88	0.30	0.03	1.189	29.884
110.35	4.35	37.64	4.58	2.30	0.02	9.66	0.32	0.03	1.250	29.770
120.42	4.37	37.63	4.51	2.28	0.04	10.42	0.33	0.03	1.397	31.612

H_2O_2 Synthesis Data Sheet

Entry No. 52 (Exp. T009) Employed in: Fig. 9

Catalyst, Additives			Reaction conditions		Gas feed rate (sccm)				
Name	Conc.	(Unit)	T_0 (℃)	28.4		H_2	O_2	N_2	Sum
Pt-PVP	1.04	(mg/L)	T (℃)	30.1	Set	5.00	20.00	25.00	50.00
			P_0 (hPa)	993.6	Calibrated	5.04	18.51	24.85	48.39
			P (hPa)	1001.5	Determination of final $[H_2O_2]$		Sample (g)	Absorbance (—)	$[H_2O_2]$ (mmol L^{-1})
			Agitation (rpm)	1200					
							1.822	0.003	0.06
Comment: Catalyst activation: H_2 gas 20 sccm at 303 K for 40 min.					Analysis of H_2O_2 formation selectivity and H_2O_2 destruction rate			S_f (—)	0.0467
								k_d[Cat] (h^{-1})	0.0203
								R^2	0.0109

GC calibration		GC count			Ratio of sensitivity (toward N_2)				Feed gas measurement	
Timing	No.	H_2	O_2	N_2	H_2		O_2			
Before reaction	1	514885	202581	221852	0.0873	0.0868	0.816	0.816	T_a (℃)	28.4
	2	515240	202303	221459	0.0871		0.816		P_0 (hPa)	993.2
	3	516002	202068	221211	0.0869		0.816		Flow	(cc/min)
After reaction	4	516783	201164	220397	0.0864		0.816		H_2	5.90
	5	516957	201232	220496	0.0864		0.816		O_2	21.69
	6	517048	201215	220479	0.0864		0.816		N_2	29.11

Time				GC count			$t_{correct.}$	Outlet flow (sccm)		Conversion(%)	
H	M	S	min.	H_2	O_2	N_2	(min)	H_2	O_2	H_2	O_2
17	47	34	4.0	309041	119363	289920	0.00	3.44	17.67	31.62	4.53
17	57	38	14.1	348211	189826	228922	9.81	3.48	17.70	30.87	4.40
18	7	40	24.1	361548	194816	223741	19.85	3.52	17.72	30.10	4.28
18	17	42	34.1	367702	194945	222759	29.88	3.56	17.74	29.33	4.15
18	37	48	54.2	374579	194850	222054	49.98	3.64	17.79	27.78	3.89
18	37	48	54.2	374579	194850	222054	49.98	3.64	17.79	27.78	3.89
18	47	52	64.3	377384	194731	222127	60.05	3.66	17.78	27.26	3.98
18	57	54	74.3	379826	194592	221512	70.08	3.70	17.81	26.59	3.78
19	7	58	84.4	382104	194678	221462	80.15	3.72	17.82	26.13	3.72
19	18	0	94.4	383334	194437	221151	90.18	3.74	17.83	25.79	3.70
19	28	4	104.5	385408	194657	221250	100.25	3.76	17.84	25.42	3.64
19	38	6	114.5	386225	194542	221018	110.28	3.77	17.85	25.18	3.59
19	48	10	124.6	387447	194327	220718	120.35	3.78	17.85	24.85	3.57

$t_{correct.}$	Partial pressure (kPa)		Rate (mmol L^{-1} h^{-1})		$d[H_2O_2]/dt$	$\Sigma[H_2]$	$[H_2O_2]$	S_e	$\Sigma_2/[H_2O_2]$	$\Sigma_1/[H_2O_2]$
(min)	p_{H2}	p_{O2}	r_{H2}	r_{O2}	(mmol L^{-1} h^{-1})	(mmol L^{-1})	(mmol L^{-1})	(—)	(h)	(—)
0.00	7.19	36.88	14.22	7.49	0.75	0.00	0.00		0.000	0.000
9.81	7.25	36.88	13.88	7.28	0.68	2.30	0.12	0.05	0.082	19.572
19.85	7.33	36.88	13.53	7.07	0.60	4.59	0.22	0.05	0.170	20.417
29.88	7.40	36.88	13.19	6.86	0.53	6.82	0.32	0.05	0.262	21.363
49.98	7.54	36.88	12.49	6.43	0.37	11.12	0.47	0.04	0.459	23.649
49.98	7.54	36.88	12.49	6.43	0.37	11.12	0.47	0.04	0.459	23.649
60.05	7.59	36.84	12.26	6.58	0.90	13.20	0.58	0.04	0.526	22.853
70.08	7.65	36.86	11.95	6.25	0.55	15.22	0.70	0.05	0.587	21.765
80.15	7.69	36.85	11.75	6.15	0.55	17.21	0.79	0.05	0.677	21.740
90.18	7.72	36.84	11.59	6.12	0.65	19.17	0.89	0.05	0.759	21.496
100.25	7.76	36.84	11.43	6.01	0.60	21.10	1.00	0.05	0.838	21.186
110.28	7.78	36.85	11.32	5.94	0.56	23.00	1.09	0.05	0.924	21.061
120.35	7.81	36.84	11.17	5.90	0.63	24.89	1.19	0.05	1.008	20.891

H_2O_2 Synthesis Data Sheet

Entry No. 53 (Exp. T011) Employed in: Fig. 9

Catalyst, Additives			Reaction conditions		Gas feed rate (sccm)				
Name	Conc.	(Unit)	T_0 (℃)	27.5		H_2	O_2	N_2	Sum
Pt-PVP	1.04	(mg/L)	T (℃)	30.2	Set	7.50	20.00	22.50	50.00
			P_0 (hPa)	999.7	Calibrated	7.57	18.52	22.26	48.34
			P (hPa)	1007.3	Determination of final $[H_2O_2]$		Sample (g)	Absorbance (—)	$[H_2O_2]$ (mmol L^{-1})
			Agitation (rpm)	1200					
							1.533	0.013	0.29
Comment: Catalyst activation: H_2 gas 20 sccm at 303 K for 40 min.					Analysis of H_2O_2 formation selectivity and H_2O_2 destruction rate			S_f (—)	0.0431
								k_d[Cat] (h^{-1})	0.2462
								R^2	0.9228

GC calibration		GC count			Ratio of sensitivity (toward N_2)				Feed gas measurement	
Timing	No.	H_2	O_2	N_2	H_2		O_2			
Before reaction	1	768698	201690	198810	0.0879	0.0879	0.820	0.819	T_a (℃)	27.1
	2	767725	201887	198798	0.0880		0.819		P_0 (hPa)	1002.1
	3	767660	201747	198746	0.0880		0.820		Flow	(cc/min)
After reaction	4	769009	201883	198806	0.0879		0.819		H_2	8.72
	5	769153	201912	198667	0.0878		0.819		O_2	21.34
	6	769162	202032	198781	0.0879		0.819		N_2	25.65

Time				GC count			$t_{correct.}$	Outlet flow (sccm)		Conversion(%)	
H	M	S	min.	H_2	O_2	N_2	(min)	H_2	O_2	H_2	O_2
16	2	16	4.0	412289	118752	282684	0.00	4.90	17.12	35.30	7.53
16	12	18	14.0	510184	190327	215348	9.60	4.95	17.16	34.54	7.35
16	22	22	24.1	529337	195761	208876	19.67	5.01	17.19	33.74	7.17
16	32	24	34.1	539381	196564	208123	29.70	5.07	17.22	32.97	7.00
16	42	28	44.2	545061	196453	207430	39.77	5.14	17.27	32.04	6.74
16	52	30	54.2	549663	196392	207096	49.80	5.19	17.29	31.36	6.62
17	2	32	64.3	552751	196355	206764	59.83	5.23	17.32	30.86	6.49
17	12	36	74.3	556082	196298	206543	69.90	5.27	17.33	30.37	6.42
17	22	38	84.4	559241	196395	206385	79.93	5.30	17.35	29.92	6.30
17	32	42	94.4	561660	196274	206277	90.00	5.33	17.35	29.58	6.31
17	42	44	104.5	563611	196477	206110	100.03	5.35	17.38	29.28	6.13
17	52	48	114.5	565599	196383	205923	110.10	5.37	17.39	28.97	6.09
18	2	50	124.6	566919	196207	205754	120.13	5.39	17.39	28.74	6.10

$t_{correct.}$	Partial pressure (kPa)		Rate (mmol L^{-1} h^{-1})		d$[H_2O_2]$/dt	$\Sigma[H_2]$	$[H_2O_2]$	S_f	$\Sigma_2/[H_2O_2]$	$\Sigma_1/[H_2O_2]$
(min)	p_{H2}	p_{O2}	r_{H2}	r_{O2}	(mmol L^{-1} h^{-1})	(mmol L^{-1})	(mmol L^{-1})	(—)	(h)	(—)
0.00	10.67	37.31	23.85	12.45	1.06	0.00	0.00		0.000	0.000
9.60	10.77	37.31	23.33	12.16	0.98	3.77	0.16	0.04	0.080	23.084
19.67	10.88	37.31	22.79	11.85	0.90	7.64	0.32	0.04	0.167	23.759
29.70	10.98	37.30	22.28	11.57	0.87	11.41	0.47	0.04	0.255	24.288
39.77	11.11	37.30	21.65	11.15	0.65	15.10	0.60	0.04	0.351	25.291
49.80	11.20	37.29	21.19	10.95	0.71	18.68	0.71	0.04	0.449	26.308
59.83	11.27	37.29	20.85	10.73	0.60	22.19	0.82	0.04	0.545	27.078
69.90	11.33	37.28	20.52	10.61	0.70	25.66	0.93	0.04	0.639	27.636
79.93	11.39	37.28	20.21	10.41	0.61	29.07	1.04	0.04	0.730	28.015
90.00	11.44	37.26	19.98	10.43	0.87	32.44	1.16	0.04	0.811	27.932
100.03	11.48	37.28	19.78	10.14	0.50	35.77	1.28	0.04	0.898	28.037
110.10	11.52	37.27	19.57	10.07	0.58	39.07	1.37	0.03	1.001	28.598
120.13	11.55	37.26	19.42	10.09	0.75	42.33	1.48	0.03	1.087	28.649

H_2O_2 Synthesis Data Sheet

Entry No. 54 (Exp. T008) Employed in: Fig. 9

Catalyst, Additives			Reaction conditions		Gas feed rate (sccm)				
Name	Conc.	(Unit)	T_0 (℃)	24.7		H_2	O_2	N_2	Sum
Pt-PVP	1.04	(mg/L)	T (℃)	30.1	Set	10.00	20.00	20.00	50.00
			P_0 (hPa)	1008.5	Calibrated	9.99	18.45	19.96	48.40
			P (hPa)	1015.8	Determination of final $[H_2O_2]$		Sample (g)	Absorbance (—)	$[H_2O_2]$ (mmol L^{-1})
			Agitation (rpm)	1200					
							1.306	0.016	0.42
Comment: Catalyst activation: H_2 gas 20 sccm at 303 K for 40 min.					Analysis of H_2O_2 formation selectivity and H_2O_2 destruction rate			S_f (—)	0.0527
								k_d[Cat] (h^{-1})	0.2651
								R^2	0.9480

GC calibration		GC count			Ratio of sensitivity (toward N_2)				Feed gas measurement	
Timing	No.	H_2	O_2	N_2	H_2		O_2			
Before reaction	1	1015268	204903	178881	0.0882	0.0881	0.807	0.807	T_a (℃)	24.8
	2	1014446	204860	178836	0.0883		0.807		P_0 (hPa)	1008.4
	3	1014743	204673	178640	0.0881		0.807		Flow	(cc/min)
After reaction	4	1013004	203910	177895	0.0879		0.806		H_2	11.30
	5	1013348	203980	177912	0.0879		0.806		O_2	20.86
	6	1012869	204009	177999	0.0880		0.806		N_2	22.57

Time				GC count			$t_{correct.}$	Outlet flow (sccm)		Conversion(%)	
H	M	S	min.	H_2	O_2	N_2	(min)	H_2	O_2	H_2	O_2
14	59	30	4.0	524077	116123	281425	0.00	6.06	16.37	39.31	11.23
15	9	34	14.1	661919	193700	205747	9.41	6.15	16.42	38.48	10.96
15	19	36	24.1	690949	200452	193732	19.44	6.24	16.48	37.59	10.67
15	29	38	34.1	703613	200881	195665	29.48	6.32	16.53	36.74	10.41
15	39	42	44.2	712272	200793	194765	39.54	6.43	16.59	35.67	10.03
15	49	44	54.2	718895	200813	194328	49.58	6.50	16.63	34.93	9.82
15	59	48	64.3	723540	200417	193579	59.64	6.57	16.67	34.25	9.65
16	9	50	74.3	727647	200528	193370	69.68	6.61	16.69	33.81	9.50
16	19	54	84.4	731111	200358	192910	79.74	6.66	16.72	33.33	9.37
16	29	56	94.4	734652	200254	192523	89.78	6.71	16.74	32.88	9.23
16	40	0	104.5	737373	200164	192272	99.84	6.74	16.76	32.54	9.15
16	50	2	114.5	739320	200052	192025	109.88	6.77	16.77	32.27	9.09
17	0	6	124.6	740712	199700	191679	119.94	6.79	16.77	32.02	9.08

$t_{correct.}$	Partial pressure (kPa)		Rate (mmol L^{-1} h^{-1})		$d[H_2O_2]/dt$	$\Sigma[H_2]$	$[H_2O_2]$	S_e	$\Sigma_2/[H_2O_2]$	$\Sigma_1/[H_2O_2]$
(min)	p_{H2}	p_{O2}	r_{H2}	r_{O2}	(mmol L^{-1} h^{-1})	(mmol L^{-1})	(mmol L^{-1})	(—)	(h)	(—)
0.00	13.92	37.59	35.07	18.49	1.91	0.00	0.00		0.000	0.000
9.41	14.07	37.59	34.33	18.05	1.77	5.44	0.29	0.05	0.078	18.893
19.44	14.22	37.58	33.53	17.57	1.62	11.12	0.57	0.05	0.165	19.475
29.48	14.37	37.58	32.78	17.14	1.50	16.66	0.83	0.05	0.255	20.035
39.54	14.56	37.58	31.82	16.53	1.23	22.08	1.06	0.05	0.349	20.816
49.58	14.69	37.57	31.16	16.18	1.20	27.35	1.26	0.05	0.447	21.644
59.64	14.81	37.56	30.56	15.90	1.24	32.52	1.47	0.05	0.541	22.162
69.68	14.88	37.56	30.16	15.65	1.15	37.60	1.67	0.04	0.634	22.560
79.74	14.96	37.55	29.74	15.42	1.11	42.63	1.86	0.04	0.728	22.965
89.78	15.04	37.55	29.33	15.20	1.07	47.56	2.04	0.04	0.823	23.328
99.84	15.10	37.54	29.03	15.07	1.12	52.46	2.22	0.04	0.915	23.599
109.88	15.15	37.53	28.79	14.97	1.14	57.29	2.41	0.04	1.004	23.757
119.94	15.19	37.51	28.57	14.96	1.35	62.11	2.62	0.04	1.085	23.701

H_2O_2 Synthesis Data Sheet

Entry No. 55 (Exp. T010) Employed in: Fig. 9

Catalyst, Additives			Reaction conditions		Gas feed rate (sccm)				
Name	Conc.	(Unit)	T_0 (℃)	27.0		H_2	O_2	N_2	Sum
Pt-PVP	1.04	(mg/L)	T (℃)	30.2	Set	15.00	20.00	15.00	50.00
			P_0 (hPa)	996.7	Calibrated	15.06	18.48	14.98	48.52
			P (hPa)	1003.2	Determination of final $[H_2O_2]$		Sample (g)	Absorbance (—)	$[H_2O_2]$ (mmol L^{-1})
			Agitation (rpm)	1200					
							1.496	0.025	0.58
Comment: Catalyst activation: H_2 gas 20 sccm at 303 K for 40 min.					Analysis of H_2O_2 formation selectivity and H_2O_2 destruction rate			S_f (—)	0.0338
								k_d[Cat] (h^{-1})	0.1680
								R^2	0.9148

GC calibration		GC count			Ratio of sensitivity (toward N_2)				Feed gas measurement	
Timing	No.	H_2	O_2	N_2	H_2		O_2			
Before reaction	1	1467031	202352	133301	0.0913	0.0910	0.813	0.811	T_a (℃)	26.8
	2	1467616	202342	133117	0.0912		0.812		P_0 (hPa)	996.8
	3	1467786	202279	133047	0.0911		0.811		Flow	(cc/min)
After reaction	4	1466496	201554	132336	0.0907		0.810		H_2	17.42
	5	1467028	201472	132394	0.0907		0.811		O_2	21.38
	6	1466520	201419	132322	0.0907		0.810		N_2	17.33

Time				GC count			$t_{correct.}$	Outlet flow (sccm)		Conversion(%)	
H	M	S	min.	H_2	O_2	N_2	(min)	H_2	O_2	H_2	O_2
10	33	10	4.0	707522	112721	260580	0.00	8.29	14.98	44.92	18.93
10	43	12	14.0	955609	191229	173606	8.97	8.41	15.04	44.16	18.59
10	53	16	24.1	997953	199389	162562	19.03	8.54	15.12	43.30	18.20
11	3	18	34.1	1018032	200125	160156	29.07	8.66	15.18	42.48	17.84
11	13	22	44.2	1028540	199804	158969	39.13	8.82	15.27	41.45	17.36
11	23	24	54.2	1036434	199590	158196	49.17	8.93	15.33	40.72	17.04
11	33	26	64.3	1043394	199482	157668	59.20	9.02	15.37	40.12	16.81
11	43	30	74.3	1047964	199274	157080	69.27	9.09	15.42	39.63	16.59
11	53	32	84.4	1051579	199203	156677	79.30	9.15	15.45	39.27	16.40
12	3	36	94.4	1054764	199202	156562	89.37	9.18	15.46	39.04	16.34
12	13	38	104.5	1059064	199162	156338	99.40	9.23	15.48	38.70	16.24
12	23	42	114.5	1061531	199014	156038	109.47	9.27	15.50	38.44	16.14
12	33	44	124.6	1065845	199141	155886	119.50	9.32	15.52	38.13	16.00

$t_{correct.}$	Partial pressure (kPa)		Rate (mmol L^{-1} h^{-1})		d$[H_2O_2]$/dt	$\Sigma[H_2]$	$[H_2O_2]$	S_e	$\Sigma_2/[H_2O_2]$	$\Sigma_1/[H_2O_2]$
(min)	p_{H2}	p_{O2}	r_{H2}	r_{O2}	(mmol L^{-1} h^{-1})	(mmol L^{-1})	(mmol L^{-1})	(—)	(h)	(—)
0.00	20.83	37.62	60.40	31.24	2.09	0.00	0.00		0.000	0.000
8.97	21.02	37.61	59.37	30.68	1.98	8.95	0.30	0.03	0.075	29.393
19.03	21.23	37.59	58.22	30.04	1.86	18.81	0.63	0.03	0.161	30.013
29.07	21.43	37.57	57.11	29.44	1.76	28.46	0.93	0.03	0.249	30.609
39.13	21.68	37.56	55.73	28.64	1.56	37.92	1.21	0.03	0.340	31.391
49.17	21.86	37.54	54.74	28.13	1.51	47.16	1.46	0.03	0.433	32.202
59.20	22.01	37.52	53.94	27.74	1.55	56.25	1.72	0.03	0.523	32.702
69.27	22.12	37.51	53.28	27.37	1.46	65.24	1.97	0.03	0.613	33.082
79.30	22.21	37.51	52.79	27.07	1.34	74.11	2.21	0.03	0.707	33.590
89.37	22.26	37.50	52.48	26.97	1.45	82.94	2.44	0.03	0.799	33.992
99.40	22.35	37.48	52.03	26.80	1.56	91.68	2.69	0.03	0.884	34.066
109.47	22.41	37.47	51.68	26.63	1.58	100.38	2.95	0.03	0.965	33.972
119.50	22.48	37.46	51.26	26.41	1.55	108.99	3.22	0.03	1.047	33.877

H_2O_2 Synthesis Data Sheet

Entry No. 56 (Exp. T020) Employed in: Fig. 9

Catalyst, Additives			Reaction conditions		Gas feed rate (sccm)				
Name	Conc.	(Unit)	T_0 (℃)	27.5		H_2	O_2	N_2	Sum
Pt-PVP	1.04	(mg/L)	T (℃)	30.2	Set	5.00	20.00	25.00	50.00
			P_0 (hPa)	1008.8	Calibrated	5.19	18.44	24.71	48.34
H_2SO_4	0.01	(N)	P (hPa)	1016.7	Determination of final $[H_2O_2]$		Sample (g)	Absorbance (—)	$[H_2O_2]$ (mmol L^{-1})
			Agitation (rpm)	1199					
							1.759	0.016	0.31
Comment: Catalyst activation: H_2 gas 20 sccm at 303 K for 40 min.					Analysis of H_2O_2 formation selectivity and H_2O_2 destruction rate			S_f (—)	0.0238
								k_d[Cat] (h^{-1})	1.0077
								R^2	0.7457

GC calibration		GC count			Ratio of sensitivity (toward N_2)				Feed gas measurement	
Timing	No.	H_2	O_2	N_2	H_2		O_2			
Before reaction	1	515986	200384	219114	0.0891	0.0888	0.816	0.817	T_a (℃)	28.9
	2	516610	200503	219173	0.0890		0.816		P_0 (hPa)	1008.0
	3	516494	200047	218745	0.0889		0.816		Flow	(cc/min)
After reaction	4	518385	199969	218990	0.0887		0.817		H_2	6.00
	5	518781	200003	218972	0.0886		0.817		O_2	21.34
	6	518964	200305	219166	0.0886		0.817		N_2	28.59

Time				GC count			$t_{correct.}$	Outlet flow (sccm)		Conversion(%)	
H	M	S	min.	H_2	O_2	N_2	(min)	H_2	O_2	H_2	O_2
17	41	44	4.0	282772	118276	290872	0.00	3.49	17.57	32.70	4.71
17	51	48	14.1	345704	188538	228058	9.73	3.53	17.60	31.95	4.59
18	1	50	24.1	358711	193661	222806	19.77	3.57	17.62	31.18	4.46
18	11	54	34.2	365054	194211	222119	29.83	3.61	17.64	30.44	4.34
18	21	56	44.2	369450	194403	221921	39.87	3.65	17.68	29.54	4.16
18	32	0	54.3	372456	194347	221666	49.93	3.69	17.69	28.89	4.08
18	42	2	64.3	375082	194290	221374	59.97	3.72	17.71	28.29	3.98
18	52	6	74.4	377109	194328	221336	70.03	3.74	17.72	27.89	3.95
19	2	8	84.4	379154	194374	221304	80.07	3.76	17.72	27.49	3.91
19	12	12	94.5	380867	194153	221117	90.13	3.78	17.72	27.10	3.94
19	22	14	104.5	382404	194393	221061	100.17	3.80	17.74	26.79	3.79
19	32	18	114.6	381321	193530	220281	110.23	3.80	17.73	26.74	3.88
19	42	20	124.6	384256	193999	220671	120.27	3.82	17.74	26.31	3.82

$t_{correct.}$	Partial pressure (kPa)		Rate (mmol L^{-1} h^{-1})		d$[H_2O_2]$/dt	$\Sigma[H_2]$	$[H_2O_2]$	S_e	$\Sigma_2/[H_2O_2]$	$\Sigma_1/[H_2O_2]$
(min)	p_{H2}	p_{O2}	r_{H2}	r_{O2}	(mmol L^{-1} h^{-1})	(mmol L^{-1})	(mmol L^{-1})	(—)	(h)	(—)
0.00	7.43	37.40	15.14	7.76	0.39	0.00	0.00		0.000	0.000
9.73	7.50	37.40	14.79	7.56	0.32	2.43	0.06	0.02	0.081	42.516
19.77	7.58	37.40	14.44	7.34	0.25	4.87	0.10	0.02	0.174	46.761
29.83	7.65	37.40	14.10	7.15	0.21	7.27	0.14	0.02	0.273	51.099
39.87	7.73	37.41	13.68	6.86	0.03	9.59	0.16	0.02	0.396	59.139
49.93	7.80	37.40	13.38	6.72	0.06	11.86	0.17	0.01	0.542	69.754
59.97	7.85	37.40	13.10	6.56	0.01	14.07	0.18	0.01	0.686	79.761
70.03	7.89	37.39	12.92	6.50	0.08	16.25	0.18	0.01	0.820	88.037
80.07	7.93	37.38	12.73	6.44	0.15	18.40	0.20	0.01	0.901	90.174
90.13	7.97	37.36	12.55	6.49	0.42	20.52	0.25	0.01	0.882	81.473
100.17	8.00	37.38	12.40	6.25	0.09	22.60	0.29	0.01	0.908	76.627
110.23	8.01	37.36	12.38	6.39	0.41	24.68	0.34	0.01	0.951	73.205
120.27	8.05	37.35	12.18	6.29	0.40	26.74	0.40	0.02	0.945	66.023

H_2O_2 Synthesis Data Sheet

Entry No. 57 (Exp. T022) Employed in: Fig. 9

Catalyst, Additives			Reaction conditions		Gas feed rate (sccm)				
Name	Conc.	(Unit)	T_0 (℃)	27.1		H_2	O_2	N_2	Sum
Pt-PVP	1.04	(mg/L)	T (℃)	30.3	Set	7.50	20.00	22.50	50.00
			P_0 (hPa)	1007.1	Calibrated	7.39	18.56	22.37	48.32
H_2SO_4	0.01	(N)	P (hPa)	1014.7	Determination of final $[H_2O_2]$		Sample (g)	Absorbance (—)	$[H_2O_2]$ (mmol L^{-1})
			Agitation (rpm)	1201					
							1.973	0.027	0.47
Comment: Catalyst activation: H_2 gas 20 sccm at 303 K for 40 min.					Analysis of H_2O_2 formation selectivity and H_2O_2 destruction rate			S_f (—)	0.0720
								k_d[Cat] (h^{-1})	0.0650
								R^2	0.7913

GC calibration		GC count			Ratio of sensitivity (toward N_2)				Feed gas measurement	
Timing	No.	H_2	O_2	N_2	H_2		O_2			
Before reaction	1	766204	201428	197929	0.0854	0.0853	0.815	0.815	T_a (℃)	27.1
	2	766117	201323	197724	0.0853		0.815		P_0 (hPa)	1007.7
	3	766115	201379	197869	0.0854		0.815		Flow	(cc/min)
After reaction	4	763416	200693	197092	0.0853		0.815		H_2	8.47
	5	763365	200422	196981	0.0853		0.816		O_2	21.27
	6	763314	200653	197025	0.0853		0.815		N_2	25.63

Time				GC count			$t_{correct.}$	Outlet flow (sccm)		Conversion(%)	
H	M	S	min.	H_2	O_2	N_2	(min)	H_2	O_2	H_2	O_2
15	59	40	4.0	370607	119655	283876	0.00	4.77	17.16	35.47	7.58
16	9	44	14.1	509616	189659	214229	9.59	4.81	17.18	34.97	7.46
16	19	46	24.1	524227	195260	208158	19.63	4.85	17.20	34.46	7.34
16	29	50	34.2	530133	195740	207251	29.69	4.88	17.22	33.96	7.22
16	39	52	44.2	533811	195621	206815	39.73	4.93	17.25	33.36	7.08
16	49	56	54.3	536310	195464	206403	49.79	4.96	17.27	32.92	6.97
16	59	58	64.3	537830	195061	205907	59.83	4.98	17.28	32.57	6.94
17	10	2	74.4	540281	195073	205712	69.89	5.01	17.29	32.19	6.85
17	20	4	84.4	542618	195029	205571	79.93	5.04	17.30	31.85	6.80
17	30	8	94.5	544950	195428	205851	89.99	5.05	17.31	31.65	6.74
17	40	10	104.5	546644	195578	205752	100.03	5.07	17.33	31.41	6.62
17	50	12	114.5	547977	195384	205573	110.06	5.09	17.33	31.18	6.63
18	0	16	124.6	547782	195035	204990	120.13	5.10	17.35	31.01	6.54

$t_{correct.}$	Partial pressure (kPa)		Rate (mmol L^{-1} h^{-1})		$d[H_2O_2]/dt$	$\Sigma[H_2]$	$[H_2O_2]$	S_e	$\Sigma_2/[H_2O_2]$	$\Sigma_1/[H_2O_2]$
(min)	p_{H2}	p_{O2}	r_{H2}	r_{O2}	(mmol L^{-1} h^{-1})	(mmol L^{-1})	(mmol L^{-1})	(—)	(h)	(—)
0.00	10.47	37.66	23.41	12.57	1.73	0.00	0.00		0.000	0.000
9.59	10.54	37.65	23.08	12.37	1.66	3.72	0.27	0.07	0.080	13.735
19.63	10.61	37.65	22.74	12.17	1.59	7.55	0.54	0.07	0.165	13.918
29.69	10.67	37.65	22.42	11.97	1.52	11.34	0.80	0.07	0.252	14.112
39.73	10.75	37.65	22.02	11.74	1.45	15.05	1.05	0.07	0.340	14.308
49.79	10.81	37.65	21.73	11.55	1.38	18.72	1.29	0.07	0.430	14.515
59.83	10.86	37.64	21.49	11.50	1.51	22.34	1.53	0.07	0.516	14.586
69.89	10.91	37.64	21.25	11.35	1.44	25.92	1.78	0.07	0.600	14.573
79.93	10.96	37.63	21.02	11.27	1.52	29.46	2.03	0.07	0.684	14.534
89.99	10.98	37.63	20.89	11.17	1.44	32.97	2.28	0.07	0.768	14.488
100.03	11.01	37.64	20.73	10.98	1.22	36.45	2.50	0.07	0.859	14.589
110.06	11.04	37.63	20.58	10.99	1.41	39.91	2.72	0.07	0.950	14.680
120.13	11.06	37.64	20.47	10.83	1.20	43.35	2.94	0.07	1.041	14.760

H_2O_2 Synthesis Data Sheet

Entry No. 58 (Exp. T027) Employed in: Fig. 9

Catalyst, Additives			Reaction conditions		Gas feed rate (sccm)				
Name	Conc.	(Unit)	T_0 (℃)	27.0		H_2	O_2	N_2	Sum
Pt-PVP	1.04	(mg/L)	T (℃)	30.3	Set	10.00	17.50	22.50	50.00
			P_0 (hPa)	999.5	Calibrated	9.98	16.22	22.37	48.58
H_2SO_4	0.01	(N)	P (hPa)	1006.7	Determination of final $[H_2O_2]$		Sample (g)	Absorbance (—)	$[H_2O_2]$ (mmol L^{-1})
			Agitation (rpm)	1201					
							1.641	0.028	0.59
Comment: Catalyst activation: H_2 gas 20 sccm at 303 K for 40 min.					Analysis of H_2O_2 formation selectivity and H_2O_2 destruction rate			S_f (—)	0.0494
								k_d[Cat] (h^{-1})	-0.0379
								R^2	0.3051

GC calibration		GC count			Ratio of sensitivity (toward N_2)				Feed gas measurement	
Timing	No.	H_2	O_2	N_2	H_2		O_2			
Before reaction	1	999182	175146	196622	0.0878	0.0878	0.814	0.814	T_a (℃)	27.0
	2	999470	175244	196618	0.0878		0.814		P_0 (hPa)	999.4
	3	999253	175196	196504	0.0877		0.813		Flow	(cc/min)
After reaction	4	995875	174320	195749	0.0877		0.814		H_2	11.53
	5	996381	174698	195926	0.0877		0.813		O_2	18.74
	6	996149	174493	195845	0.0877		0.814		N_2	25.84

Time				GC count			$t_{correct.}$	Outlet flow (sccm)		Conversion(%)	
H	M	S	min.	H_2	O_2	N_2	(min)	H_2	O_2	H_2	O_2
15	32	8	4.0	479460	102594	288156	0.00	5.79	14.03	42.00	13.53
15	42	12	14.1	628233	162701	225261	9.41	5.84	14.05	41.46	13.38
15	52	14	24.1	649983	168012	218920	19.45	5.90	14.08	40.90	13.22
16	2	18	34.2	660322	168572	217680	29.51	5.96	14.10	40.34	13.10
16	12	0	43.9	664622	168496	216878	39.21	6.02	14.15	39.73	12.82
16	22	22	54.2	669486	168314	216534	49.58	6.07	14.15	39.20	12.77
16	32	26	64.3	671704	168427	216008	59.65	6.10	14.20	38.85	12.50
16	42	28	74.3	672934	168082	215597	69.68	6.13	14.19	38.62	12.51
16	52	32	84.4	674966	168172	215325	79.75	6.15	14.22	38.35	12.36
17	2	34	94.4	677969	168160	215128	89.78	6.19	14.23	38.02	12.28
17	12	38	104.5	680056	168257	215032	99.85	6.21	14.25	37.80	12.19
17	22	40	114.5	681591	168119	214673	109.88	6.23	14.26	37.56	12.12
17	32	44	124.6	680742	168001	214570	119.95	6.23	14.26	37.61	12.14

$t_{correct.}$	Partial pressure (kPa)		Rate (mmol L^{-1} h^{-1})		$d[H_2O_2]/dt$	$\Sigma[H_2]$	$[H_2O_2]$	S_e	$\Sigma_2/[H_2O_2]$	$\Sigma_1/[H_2O_2]$
(min)	p_{H2}	p_{O2}	r_{H2}	r_{O2}	(mmol L^{-1} h^{-1})	(mmol L^{-1})	(mmol L^{-1})	(—)	(h)	(—)
0.00	13.23	32.06	37.43	19.60	1.76	0.00	0.00		0.000	0.000
9.41	13.33	32.06	36.96	19.38	1.80	5.84	0.28	0.05	0.078	20.867
19.45	13.43	32.06	36.45	19.15	1.84	11.97	0.58	0.05	0.161	20.484
29.51	13.53	32.05	35.96	18.98	1.99	18.05	0.91	0.05	0.242	19.912
39.21	13.64	32.07	35.41	18.57	1.72	23.82	1.21	0.05	0.323	19.741
49.58	13.74	32.04	34.94	18.50	2.07	29.90	1.53	0.05	0.409	19.489
59.65	13.80	32.08	34.62	18.11	1.60	35.73	1.84	0.05	0.494	19.402
69.68	13.84	32.06	34.42	18.13	1.84	41.50	2.13	0.05	0.583	19.496
79.75	13.88	32.08	34.19	17.90	1.62	47.26	2.42	0.05	0.671	19.540
89.78	13.94	32.07	33.89	17.79	1.70	52.95	2.70	0.05	0.761	19.643
99.85	13.98	32.08	33.70	17.66	1.63	58.62	2.97	0.05	0.849	19.705
109.88	14.02	32.08	33.48	17.56	1.63	64.24	3.25	0.05	0.938	19.778
119.95	14.02	32.08	33.52	17.58	1.65	69.86	3.52	0.05	1.026	19.828

H_2O_2 Synthesis Data Sheet

Entry No. 59 (Exp. T019) Employed in: Fig. 9

Catalyst, Additives			Reaction conditions		Gas feed rate (sccm)				
Name	Conc.	(Unit)	T_0 (℃)	28.7		H_2	O_2	N_2	Sum
Pt-PVP	1.04	(mg/L)	T (℃)	30.4	Set	10.00	20.00	20.00	50.00
			P_0 (hPa)	1011.0	Calibrated	10.17	18.56	20.02	48.74
H_2SO_4	0.01	(N)	P (hPa)	1018.4	Determination of final $[H_2O_2]$		Sample (g)	Absorbance (—)	$[H_2O_2]$ (mmol L^{-1})
			Agitation (rpm)	1198					
							1.822	0.038	0.72
Comment: Catalyst activation: H_2 gas 20 sccm at 303 K for 40 min.					Analysis of H_2O_2 formation selectivity and H_2O_2 destruction rate			S_f (—)	0.0414
								k_d[Cat] (h^{-1})	0.1319
								R^2	0.9071

GC calibration		GC count			Ratio of sensitivity (toward N_2)				Feed gas measurement	
Timing	No.	H_2	O_2	N_2	H_2		O_2			
Before reaction	1	996645	199425	175476	0.0894	0.0891	0.816	0.816	T_a (℃)	29.1
	2	996941	199395	175339	0.0893		0.815		P_0 (hPa)	1010.9
	3	997308	199253	175350	0.0893		0.816		Flow	(cc/min)
After reaction	4	995860	198101	174466	0.0890		0.816		H_2	11.74
	5	996842	198486	174636	0.0890		0.816		O_2	21.43
	6	997342	198496	174707	0.0890		0.816		N_2	23.12

Time				GC count			$t_{correct.}$	Outlet flow (sccm)		Conversion(%)	
H	M	S	min.	H_2	O_2	N_2	(min)	H_2	O_2	H_2	O_2
17	39	16	4.0	502789	120532	267211	0.00	6.37	16.58	37.38	10.66
17	49	20	14.1	671597	187588	196597	9.46	6.43	16.61	36.74	10.47
17	59	22	24.1	684039	193213	191033	19.49	6.50	16.65	36.07	10.27
18	9	26	34.2	696496	193539	189480	29.56	6.56	16.68	35.47	10.12
18	19	28	44.2	703628	193398	188657	39.59	6.66	16.74	34.52	9.79
18	29	32	54.3	707982	193496	188591	49.66	6.70	16.75	34.10	9.71
18	39	34	64.3	712145	193641	188242	59.69	6.75	16.80	33.59	9.48
18	49	38	74.4	715039	193704	188213	69.76	6.78	16.81	33.31	9.43
18	59	40	84.4	727471	193853	187454	79.79	6.93	16.89	31.87	9.00
19	9	44	94.5	729140	193591	187147	89.86	6.95	16.89	31.60	8.97
19	19	46	104.5	731591	193635	187087	99.89	6.98	16.90	31.35	8.92
19	29	50	114.6	731911	193472	186873	109.96	6.99	16.91	31.24	8.89
19	39	52	124.6	730170	192650	186011	119.99	7.01	16.91	31.09	8.86

$t_{correct.}$	Partial pressure (kPa)		Rate (mmol L^{-1} h^{-1})		d$[H_2O_2]$/dt	$\Sigma[H_2]$	$[H_2O_2]$	S_e	$\Sigma_2/[H_2O_2]$	$\Sigma_1/[H_2O_2]$
(min)	p_{H2}	p_{O2}	r_{H2}	r_{O2}	(mmol L^{-1} h^{-1})	(mmol L^{-1})	(mmol L^{-1})	(—)	(h)	(—)
0.00	14.46	37.66	33.93	17.66	1.40	0.00	0.00		0.000	0.000
9.46	14.57	37.65	33.35	17.35	1.35	5.30	0.22	0.04	0.079	24.459
19.49	14.69	37.64	32.73	17.02	1.31	10.83	0.44	0.04	0.164	24.635
29.56	14.80	37.63	32.19	16.76	1.32	16.27	0.66	0.04	0.249	24.642
39.59	14.96	37.63	31.34	16.22	1.10	21.59	0.86	0.04	0.338	25.011
49.66	15.04	37.61	30.95	16.09	1.23	26.81	1.06	0.04	0.428	25.323
59.69	15.12	37.63	30.48	15.70	0.92	31.95	1.24	0.04	0.521	25.796
69.76	15.18	37.62	30.23	15.63	1.03	37.04	1.40	0.04	0.618	26.429
79.79	15.42	37.60	28.93	14.90	0.88	41.99	1.56	0.04	0.714	26.895
89.86	15.47	37.59	28.68	14.86	1.04	46.82	1.72	0.04	0.807	27.185
99.89	15.52	37.58	28.46	14.78	1.10	51.60	1.90	0.04	0.890	27.138
109.96	15.54	37.58	28.36	14.73	1.11	56.36	2.09	0.04	0.971	27.008
119.99	15.56	37.57	28.22	14.68	1.14	61.09	2.27	0.04	1.051	26.855

H_2O_2 Synthesis Data Sheet

Entry No. 60 (Exp. T023) Employed in: Fig. 9

Catalyst, Additives			Reaction conditions		Gas feed rate (sccm)				
Name	Conc.	(Unit)	T_0 (℃)	26.4		H_2	O_2	N_2	Sum
Pt-PVP	1.04	(mg/L)	T (℃)	30.2	Set	12.50	20.00	17.50	50.00
			P_0 (hPa)	994.8	Calibrated	12.62	18.66	17.51	48.78
H_2SO_4	0.01	(N)	P (hPa)	1001.8	Determination of final $[H_2O_2]$		Sample (g)	Absorbance (—)	$[H_2O_2]$ (mmol L^{-1})
			Agitation (rpm)	1200					
							1.805	0.031	0.59
Comment: Catalyst activation: H_2 gas 20 sccm at 303 K for 40 min.					Analysis of H_2O_2 formation selectivity and H_2O_2 destruction rate			S_f (—)	0.0493
								k_d[Cat] (h^{-1})	0.1099
								R^2	0.9421

GC calibration		GC count			Ratio of sensitivity (toward N_2)				Feed gas measurement	
Timing	No.	H_2	O_2	N_2	H_2		O_2			
Before reaction	1	1229607	200373	153836	0.0902	0.0898	0.818	0.818	T_a (℃)	26.4
	2	1230323	200251	153693	0.0900		0.818		P_0 (hPa)	993.9
	3	1230261	200146	153533	0.0899		0.817		Flow	(cc/min)
After reaction	4	1226056	198613	152386	0.0896		0.818		H_2	14.61
	5	1226749	198712	152457	0.0896		0.818		O_2	21.60
	6	1226702	198594	152323	0.0895		0.817		N_2	20.27

Time				GC count			$t_{correct.}$	Outlet flow (sccm)		Conversion(%)	
H	M	S	min.	H_2	O_2	N_2	(min)	H_2	O_2	H_2	O_2
17	16	54	4.0	629387	120189	259721	0.00	7.60	16.02	39.79	14.13
17	26	56	14.0	826785	190108	184186	9.28	7.64	16.04	39.46	14.00
17	37	0	24.1	851246	196180	176180	19.35	7.69	16.07	39.10	13.85
17	47	2	34.1	859647	196721	174944	29.38	7.73	16.10	38.78	13.72
17	57	4	44.2	864084	196568	174431	39.41	7.79	16.13	38.28	13.53
18	7	8	54.2	865715	196432	174095	49.48	7.82	16.15	38.04	13.42
18	17	10	64.3	865759	196065	173605	59.51	7.84	16.17	37.87	13.34
18	27	14	74.3	870400	195981	173219	69.58	7.90	16.20	37.39	13.19
18	37	16	84.4	871761	195917	173144	79.61	7.92	16.20	37.27	13.18
18	47	20	94.4	872915	195911	172968	89.68	7.93	16.21	37.12	13.09
18	57	22	104.5	873904	195715	172653	99.71	7.96	16.23	36.93	13.02
19	7	26	114.5	876436	195787	172668	109.78	7.98	16.23	36.76	13.00
19	17	28	124.6	876018	195460	172144	119.81	8.00	16.25	36.60	12.88

$t_{correct.}$	Partial pressure (kPa)		Rate (mmol L^{-1} h^{-1})		$d[H_2O_2]/dt$	$\Sigma[H_2]$	$[H_2O_2]$	S_e	$\Sigma_2/[H_2O_2]$	$\Sigma_1/[H_2O_2]$
(min)	p_{H2}	p_{O2}	r_{H2}	r_{O2}	(mmol L^{-1} h^{-1})	(mmol L^{-1})	(mmol L^{-1})	(—)	(h)	(—)
0.00	17.72	37.37	44.83	23.54	2.24	0.00	0.00		0.000	0.000
9.28	17.79	37.37	44.46	23.31	2.17	6.91	0.34	0.05	0.077	20.266
19.35	17.87	37.37	44.05	23.07	2.09	14.33	0.70	0.05	0.163	20.523
29.38	17.93	37.36	43.69	22.85	2.01	21.67	1.04	0.05	0.249	20.802
39.41	18.04	37.36	43.13	22.54	1.95	28.92	1.37	0.05	0.336	21.068
49.48	18.08	37.36	42.86	22.36	1.86	36.14	1.69	0.05	0.424	21.350
59.51	18.12	37.36	42.66	22.22	1.79	43.29	2.00	0.05	0.514	21.670
69.58	18.22	37.35	42.13	21.96	1.80	50.40	2.30	0.05	0.603	21.927
79.61	18.25	37.34	41.99	21.95	1.91	57.43	2.61	0.05	0.689	22.015
89.68	18.28	37.34	41.82	21.81	1.79	64.46	2.92	0.05	0.775	22.082
99.71	18.31	37.34	41.61	21.69	1.76	71.44	3.22	0.05	0.862	22.212
109.78	18.35	37.33	41.41	21.65	1.88	78.41	3.52	0.04	0.948	22.263
119.81	18.38	37.34	41.23	21.45	1.67	85.32	3.82	0.04	1.035	22.343

H_2O_2 Synthesis Data Sheet

Entry No. 61 (Exp. T021) Employed in: Fig. 9

Catalyst, Additives			Reaction conditions		Gas feed rate (sccm)				
Name	Conc.	(Unit)	T_0 (℃)	26.2		H_2	O_2	N_2	Sum
Pt-PVP	1.04	(mg/L)	T (℃)	30.2	Set	15.00	20.00	15.00	50.00
			P_0 (hPa)	1007.8	Calibrated	15.02	18.67	15.09	48.78
H_2SO_4	0.01	(N)	P (hPa)	1014.4	Determination of final $[H_2O_2]$		Sample (g)	Absorbance (—)	$[H_2O_2]$ (mmol L^{-1})
			Agitation (rpm)	1199					
							1.762	0.038	0.74
Comment: Catalyst activation: H_2 gas 20 sccm at 303 K for 40 min.					Analysis of H_2O_2 formation selectivity and H_2O_2 destruction rate			S_f (—)	0.0580
								k_d[Cat] (h^{-1})	0.2240
								R^2	0.9296

GC calibration		GC count			Ratio of sensitivity (toward N_2)				Feed gas measurement	
Timing	No.	H_2	O_2	N_2	H_2		O_2			
Before reaction	1	1468295	203221	133216	0.0903	0.0900	0.811	0.810	T_a (℃)	25.2
	2	1467936	203495	133261	0.0903		0.810		P_0 (hPa)	1008.2
	3	1468134	203189	133008	0.0901		0.810		Flow	(cc/min)
After reaction	4	1460292	201106	131728	0.0897		0.810		H_2	17.02
	5	1461586	201302	131755	0.0897		0.809		O_2	21.16
	6	1461661	201213	131763	0.0897		0.810		N_2	17.11

Time				GC count			$t_{correct.}$	Outlet flow (sccm)		Conversion(%)	
H	M	S	min.	H_2	O_2	N_2	(min)	H_2	O_2	H_2	O_2
11	6	22	4.0	724860	118416	255548	0.00	8.72	15.33	41.91	17.86
11	16	24	14.0	1000280	191959	169332	8.98	8.76	15.36	41.63	17.70
11	26	28	24.1	1026049	199381	160120	19.05	8.81	15.40	41.32	17.52
11	36	30	34.1	1033535	200010	158467	29.08	8.86	15.43	41.02	17.34
11	46	34	44.2	1035916	199878	157966	39.15	8.90	15.47	40.69	17.13
11	56	36	54.2	1038701	199787	157593	49.18	8.95	15.50	40.39	16.98
12	6	40	64.3	1039975	199619	157206	59.25	8.98	15.52	40.17	16.84
12	16	42	74.3	1041924	199495	157094	69.28	9.01	15.53	40.02	16.83
12	26	46	84.4	1043698	199484	156862	79.35	9.03	15.55	39.83	16.72
12	36	48	94.4	1045963	199325	156560	89.38	9.07	15.56	39.58	16.62
12	46	52	104.5	1047719	198940	156187	99.45	9.11	15.57	39.34	16.58
12	56	54	114.5	1050171	198912	156051	109.48	9.14	15.58	39.14	16.52
13	6	56	124.6	1051361	199151	156021	119.51	9.15	15.60	39.06	16.41

$t_{correct.}$	Partial pressure (kPa)		Rate (mmol L^{-1} h^{-1})		$d[H_2O_2]/dt$	$\Sigma[H_2]$	$[H_2O_2]$	S_e	$\Sigma_2/[H_2O_2]$	$\Sigma_1/[H_2O_2]$
(min)	p_{H2}	p_{O2}	r_{H2}	r_{O2}	(mmol L^{-1} h^{-1})	(mmol L^{-1})	(mmol L^{-1})	(—)	(h)	(—)
0.00	21.65	38.07	56.18	29.77	3.35	0.00	0.00		0.000	0.000
8.98	21.72	38.07	55.82	29.50	3.18	8.38	0.49	0.06	0.075	17.166
19.05	21.79	38.08	55.40	29.19	2.99	17.71	1.01	0.06	0.161	17.615
29.08	21.86	38.08	54.99	28.91	2.82	26.94	1.49	0.06	0.249	18.069
39.15	21.93	38.10	54.56	28.56	2.56	36.13	1.94	0.05	0.339	18.601
49.18	22.00	38.10	54.16	28.30	2.44	45.22	2.36	0.05	0.431	19.159
59.25	22.05	38.10	53.86	28.07	2.28	54.28	2.76	0.05	0.525	19.695
69.28	22.09	38.08	53.65	28.06	2.47	63.27	3.15	0.05	0.616	20.065
79.35	22.13	38.09	53.40	27.86	2.33	72.25	3.56	0.05	0.704	20.322
89.38	22.20	38.08	53.07	27.70	2.34	81.15	3.95	0.05	0.794	20.567
99.45	22.26	38.06	52.74	27.64	2.55	90.03	4.36	0.05	0.879	20.667
109.48	22.31	38.04	52.47	27.54	2.61	98.82	4.79	0.05	0.959	20.644
119.51	22.32	38.07	52.37	27.35	2.33	107.59	5.20	0.05	1.044	20.692

H_2O_2 Synthesis Data Sheet

Entry No. 62 (Exp. Y150) Employed in: Fig. 10 Fig. 11

Catalyst, Additives			Reaction conditions		Gas feed rate (sccm)				
Name	Conc.	(Unit)	T_0 (℃)	26.0		H_2	O_2	N_2	Sum
Pd-PVP	8.33	(mg/L)	T (℃)	29.9	Set	10.00	20.00	20.00	50.00
$IrCl_3$	0.04333	(mg-Ir/L)	P_0 (hPa)	998.8	Calibrated	10.08	19.15	19.32	48.55
H_2SO_4	0.01	(N)	P (hPa)	1005.5	Determination of final $[H_2O_2]$		Sample (g)	Absorbance (—)	$[H_2O_2]$ (mmol L^{-1})
NaBr	0.001	(N)	Agitation (rpm)	1201					
							0.656	0.903	46.41
Comment: Catalyst activation: H_2 gas 20 sccm at 303 K for 40 min.					Analysis of H_2O_2 formation selectivity and H_2O_2 destruction rate			S_f (—)	0.7766
								k_d[Cat] (h^{-1})	0.3000
								R^2	0.9996

GC calibration		GC count			Ratio of sensitivity (toward N_2)				Feed gas measurement	
Timing	No.	H_2	O_2	N_2	H_2		O_2			
Before reaction	1	990777	197851	171634	0.0904	0.0904	0.860	0.860	T_a (℃)	26.0
	2	991840	197990	171771	0.0904		0.860		P_0 (hPa)	994.8
	3	991254	197949	171756	0.0904		0.860		Flow	(cc/min)
After reaction	4	993455	198196	171950	0.0903		0.860		H_2	11.64
	5	994499	198468	172204	0.0904		0.860		O_2	22.10
	6	994943	198589	172160	0.0903		0.859		N_2	22.30

Time				GC count			$t_{correct.}$	Outlet flow (sccm)		Conversion(%)	
H	M	S	min.	H_2	O_2	N_2	(min)	H_2	O_2	H_2	O_2
14	53	30	4.0	473035	113957	274264	0.00	5.28	14.88	47.63	22.27
15	3	34	14.1	598908	177292	210292	10.33	5.24	14.93	48.04	22.00
15	13	36	24.1	603480	183565	204780	20.37	5.20	14.99	48.43	21.73
15	23	40	34.2	602858	184774	204176	30.43	5.16	15.03	48.87	21.49
15	33	42	44.2	599053	185453	204004	40.47	5.13	15.10	49.15	21.14
15	43	46	54.3	592960	185876	204008	50.53	5.08	15.13	49.67	20.96
15	53	48	64.3	588889	186414	203943	60.57	5.04	15.18	50.00	20.71
16	3	52	74.4	586528	186885	203673	70.63	5.03	15.24	50.13	20.40
16	13	54	84.4	584926	187389	203629	80.67	5.02	15.28	50.26	20.17
16	23	56	94.4	586310	188065	203493	90.70	5.03	15.35	50.11	19.83
16	34	0	104.5	587826	188660	203301	100.77	5.05	15.41	49.93	19.50
16	44	2	114.5	588287	188788	202678	110.80	5.07	15.47	49.74	19.20
16	54	6	124.6	590506	189699	202788	120.87	5.08	15.54	49.58	18.85

$t_{correct.}$	Partial pressure (kPa)		Rate (mmol L^{-1} h^{-1})		$d[H_2O_2]/dt$	$\Sigma[H_2]$	$[H_2O_2]$	S_e	$\Sigma_2/[H_2O_2]$	$\Sigma_1/[H_2O_2]$
(min)	p_{H2}	p_{O2}	r_{H2}	r_{O2}	(mmol L^{-1} h^{-1})	(mmol L^{-1})	(mmol L^{-1})	(—)	(h)	(—)
0.00	12.88	36.30	42.88	38.07	33.27	0.00	0.00		0.000	0.000
10.33	12.78	36.42	43.25	37.61	31.96	7.42	5.62	0.76	0.086	1.320
20.37	12.68	36.53	43.61	37.15	30.70	14.68	10.86	0.74	0.171	1.352
30.43	12.57	36.64	44.00	36.75	29.49	22.03	15.91	0.72	0.258	1.385
40.47	12.49	36.77	44.26	36.14	28.02	29.41	20.71	0.70	0.346	1.420
50.53	12.37	36.87	44.72	35.83	26.95	36.87	25.33	0.69	0.436	1.456
60.57	12.28	36.97	45.02	35.40	25.78	44.38	29.73	0.67	0.526	1.493
70.63	12.23	37.07	45.14	34.88	24.61	51.94	33.96	0.65	0.618	1.529
80.67	12.19	37.15	45.25	34.48	23.71	59.50	38.00	0.64	0.710	1.566
90.70	12.20	37.24	45.12	33.90	22.68	67.06	41.88	0.62	0.804	1.601
100.77	12.22	37.31	44.96	33.33	21.71	74.61	45.60	0.61	0.899	1.636
110.80	12.25	37.38	44.79	32.82	20.85	82.12	49.16	0.60	0.995	1.670
120.87	12.26	37.46	44.64	32.23	19.81	89.62	52.57	0.59	1.093	1.705

H_2O_2 Synthesis Data Sheet

Entry No. 63 (Exp. Y154) Employed in: Fig. 10 Fig. 11

Catalyst, Additives			Reaction conditions		Gas feed rate (sccm)				
Name	Conc.	(Unit)	T_0 (℃)	24.1		H_2	O_2	N_2	Sum
Pd-PVP	8.33	(mg/L)	T (℃)	29.9	Set	10.00	20.00	20.00	50.00
$IrCl_3$	0.04333	(mg-Ir/L)	P_0 (hPa)	1005.0	Calibrated	9.94	18.53	19.88	48.36
H_2SO_4	0.01	(N)	P (hPa)	1011.7	Determination of final $[H_2O_2]$		Sample (g)	Absorbance (—)	$[H_2O_2]$ (mmol L^{-1})
NaBr	0.001	(N)	Agitation (rpm)	1201					
							0.589	0.747	42.75
Comment: Catalyst activation: H_2 gas 20 sccm at 303 K for 40 min.					Analysis of H_2O_2 formation selectivity and H_2O_2 destruction rate			S_f (—)	0.6810
								k_d[Cat] (h^{-1})	0.3506
								R^2	0.9993

GC calibration		GC count			Ratio of sensitivity (toward N_2)				Feed gas measurement	
Timing	No.	H_2	O_2	N_2	H_2		O_2			
Before reaction	1	991906	200339	173899	0.0877	0.0874	0.809	0.808	T_a (℃)	25.4
	2	992303	200142	173626	0.0875		0.809		P_0 (hPa)	1004.0
	3	992571	200227	173665	0.0875		0.808		Flow	(cc/min)
After reaction	4	989736	199408	172868	0.0873		0.808		H_2	11.33
	5	989510	199175	172718	0.0873		0.808		O_2	21.12
	6	989829	199203	172776	0.0873		0.808		N_2	22.66

Time				GC count			$t_{correct.}$	Outlet flow (sccm)		Conversion(%)	
H	M	S	min.	H_2	O_2	N_2	(min)	H_2	O_2	H_2	O_2
10	30	38	4.0	462065	114679	278348	0.00	5.01	14.38	49.64	22.39
10	40	42	14.1	586045	180990	215197	10.36	4.96	14.44	50.08	22.08
10	50	44	24.1	585454	186553	208099	20.39	4.92	14.50	50.52	21.77
11	0	48	34.2	581518	187590	207211	30.46	4.88	14.55	50.93	21.48
11	10	50	44.2	576135	188553	207444	40.49	4.83	14.61	51.44	21.16
11	20	54	54.3	570993	188983	207152	50.56	4.79	14.66	51.81	20.87
11	30	56	64.3	568135	189275	206696	60.59	4.78	14.72	51.94	20.57
11	41	0	74.4	566386	189538	206184	70.66	4.77	14.78	51.97	20.26
11	51	2	84.4	566990	190172	205971	80.69	4.78	14.84	51.87	19.92
12	1	6	94.5	567238	190773	205800	90.76	4.79	14.90	51.81	19.60
12	11	8	104.5	567528	190885	205139	100.79	4.81	14.96	51.63	19.29
12	21	12	114.6	567602	191241	204709	110.86	4.82	15.02	51.52	18.97
12	31	14	124.6	567766	191590	204330	120.89	4.83	15.07	51.42	18.67

$t_{correct.}$	Partial pressure (kPa)		Rate (mmol L^{-1} h^{-1})		$d[H_2O_2]/dt$	$\Sigma[H_2]$	$[H_2O_2]$	S_e	$\Sigma_2/[H_2O_2]$	$\Sigma_1/[H_2O_2]$
(min)	p_{H2}	p_{O2}	r_{H2}	r_{O2}	(mmol L^{-1} h^{-1})	(mmol L^{-1})	(mmol L^{-1})	(—)	(h)	(—)
0.00	12.36	35.49	44.06	37.04	30.03	0.00	0.00		0.000	0.000
10.36	12.24	35.62	44.46	36.53	28.60	7.64	5.06	0.66	0.086	1.510
20.39	12.13	35.75	44.85	36.03	27.21	15.11	9.73	0.64	0.172	1.553
30.46	12.03	35.87	45.21	35.53	25.86	22.66	14.18	0.63	0.259	1.598
40.49	11.90	36.01	45.66	35.01	24.36	30.26	18.38	0.61	0.348	1.647
50.56	11.80	36.13	45.99	34.53	23.08	37.95	22.36	0.59	0.439	1.697
60.59	11.76	36.23	46.11	34.04	21.97	45.65	26.12	0.57	0.531	1.747
70.66	11.73	36.32	46.13	33.53	20.93	53.39	29.72	0.56	0.624	1.796
80.69	11.74	36.41	46.04	32.95	19.86	61.09	33.13	0.54	0.719	1.844
90.76	11.73	36.49	45.99	32.42	18.86	68.82	36.38	0.53	0.815	1.891
100.79	11.75	36.56	45.83	31.92	18.00	76.49	39.46	0.52	0.912	1.938
110.86	11.76	36.64	45.74	31.39	17.04	84.17	42.40	0.50	1.011	1.985
120.89	11.77	36.72	45.64	30.89	16.14	91.81	45.18	0.49	1.111	2.032

H_2O_2 Synthesis Data Sheet

Entry No. 64 (Exp. Y160) Employed in: Fig. 10 Fig. 11

Catalyst, Additives			Reaction conditions		Gas feed rate (sccm)				
Name	Conc.	(Unit)	T_0 (℃)	20.3		H_2	O_2	N_2	Sum
Pd-PVP	8.33	(mg/L)	T (℃)	29.9	Set	16.00	20.00	20.00	56.00
$IrCl_3$	0.08667	(mg-Ir/L)	P_0 (hPa)	1001.8	Calibrated	15.88	18.61	20.03	54.52
H_2SO_4	0.01	(N)	P (hPa)	1008.5	Determination of final $[H_2O_2]$		Sample (g)	Absorbance (—)	$[H_2O_2]$ (mmol L^{-1})
NaBr	0.001	(N)	Agitation (rpm)	1196					
							0.283	0.511	60.90
Comment: Catalyst activation: H_2 gas 20 sccm at 303 K for 40 min.					Analysis of H_2O_2 formation selectivity and H_2O_2 destruction rate			S_f (—)	0.6297
								k_d[Cat] (h^{-1})	0.4946
								R^2	0.9980

GC calibration		GC count			Ratio of sensitivity (toward N_2)				Feed gas measurement	
Timing	No.	H_2	O_2	N_2	H_2		O_2			
Before reaction	1	1379673	179724	155799	0.0896	0.0894	0.806	0.805	T_a (℃)	19.3
	2	1380057	179596	155763	0.0895		0.806		P_0 (hPa)	1003.4
	3	1379693	179483	155536	0.0894		0.806		Flow	(cc/min)
After reaction	4	1376022	178867	154933	0.0893		0.805		H_2	17.56
	5	1376022	178867	154933	0.0893		0.805		O_2	20.58
	6	1376022	178867	154933	0.0893		0.805		N_2	22.14

Time				GC count			$t_{correct.}$	Outlet flow (sccm)		Conversion(%)	
H	M	S	min.	H_2	O_2	N_2	(min)	H_2	O_2	H_2	O_2
11	29	10	4.0	722361	103577	268939	0.00	7.36	11.66	53.68	37.38
11	39	14	14.1	871725	149804	217309	10.87	7.25	11.79	54.37	36.66
11	49	16	24.1	857306	156088	213160	20.90	7.15	11.91	55.01	35.99
11	59	20	34.2	840004	159010	213062	30.97	7.06	12.04	55.56	35.33
12	9	22	44.2	821602	160454	212703	41.00	6.92	12.17	56.46	34.63
12	19	26	54.3	812330	161637	212169	51.07	6.85	12.29	56.84	33.98
12	29	28	64.3	809407	162519	211514	61.10	6.85	12.39	56.87	33.42
12	39	32	74.4	808730	163427	210867	71.17	6.87	12.50	56.77	32.84
12	49	34	84.4	809691	164240	210026	81.20	6.90	12.61	56.54	32.24
12	59	38	94.5	811000	165487	209783	91.27	6.92	12.72	56.42	31.64
13	9	40	104.5	810182	165589	208161	101.30	6.97	12.83	56.13	31.07
13	19	42	114.5	811090	166421	207389	111.33	7.00	12.94	55.92	30.46
13	29	46	124.6	810855	166902	206619	121.40	7.03	13.03	55.76	30.00

$t_{correct.}$	Partial pressure (kPa)		Rate (mmol L^{-1} h^{-1})		$d[H_2O_2]/dt$	$\Sigma[H_2]$	$[H_2O_2]$	S_e	$\Sigma_2/[H_2O_2]$	$\Sigma_1/[H_2O_2]$
(min)	p_{H2}	p_{O2}	r_{H2}	r_{O2}	(mmol L^{-1} h^{-1})	(mmol L^{-1})	(mmol L^{-1})	(—)	(h)	(—)
0.00	18.20	28.84	76.12	62.13	48.15	0.00	0.00		0.000	0.000
10.87	17.92	29.15	77.10	60.93	44.76	13.87	8.41	0.61	0.091	1.649
20.90	17.66	29.44	78.01	59.82	41.63	26.84	15.64	0.58	0.177	1.717
30.97	17.43	29.72	78.79	58.72	38.64	40.00	22.37	0.56	0.266	1.788
41.00	17.08	30.05	80.07	57.56	35.05	53.28	28.53	0.54	0.358	1.867
51.07	16.90	30.31	80.61	56.48	32.35	66.76	34.19	0.51	0.453	1.953
61.10	16.85	30.49	80.64	55.54	30.44	80.24	39.44	0.49	0.549	2.035
71.17	16.84	30.66	80.51	54.58	28.65	93.76	44.39	0.47	0.646	2.112
81.20	16.86	30.82	80.19	53.58	26.96	107.20	49.04	0.46	0.744	2.186
91.27	16.85	30.99	80.02	52.59	25.16	120.64	53.42	0.44	0.844	2.258
101.30	16.90	31.13	79.60	51.63	23.67	133.98	57.50	0.43	0.945	2.330
111.33	16.92	31.29	79.30	50.63	21.96	147.27	61.31	0.42	1.048	2.402
121.40	16.94	31.41	79.08	49.86	20.65	160.55	64.89	0.40	1.154	2.474

H_2O_2 Synthesis Data Sheet

Entry No. 65 (Exp. Y159) Employed in: Fig. 10 Fig. 11

Catalyst, Additives			Reaction conditions		Gas feed rate (sccm)				
Name	Conc.	(Unit)	T_0 (℃)	26.5		H_2	O_2	N_2	Sum
Pd-PVP	8.33	(mg/L)	T (℃)	30.1	Set	17.00	20.00	20.00	57.00
$IrCl_3$	0.1734	(mg-Ir/L)	P_0 (hPa)	1005.0	Calibrated	16.82	18.68	19.81	55.31
H_2SO_4	0.01	(N)	P (hPa)	1011.6	Determination of final $[H_2O_2]$		Sample (g)	Absorbance (—)	$[H_2O_2]$ (mmol L^{-1})
NaBr	0.001	(N)	Agitation (rpm)	1198					
							0.261	0.474	61.21
Comment: Catalyst activation: H_2 gas 20 sccm at 303 K for 40 min.					Analysis of H_2O_2 formation selectivity and H_2O_2 destruction rate			S_f (—)	0.4646
								k_d[Cat] (h^{-1})	0.2530
								R^2	0.9999

GC calibration		GC count			Ratio of sensitivity (toward N_2)				Feed gas measurement	
Timing	No.	H_2	O_2	N_2	H_2		O_2			
Before reaction	1	1427811	175522	151841	0.0903	0.0904	0.816	0.817	T_a (℃)	25.8
	2	1428311	175772	152293	0.0906		0.817		P_0 (hPa)	1006.6
	3	1431953	175812	152208	0.0903		0.817		Flow	(cc/min)
After reaction	4	1427811	175522	151841	0.0903		0.816		H_2	19.16
	5	1428311	175772	152293	0.0906		0.817		O_2	21.28
	6	1431953	175812	152208	0.0903		0.817		N_2	22.56

Time				GC count			$t_{correct.}$	Outlet flow (sccm)		Conversion(%)	
H	M	S	min.	H_2	O_2	N_2	(min)	H_2	O_2	H_2	O_2
15	48	34	4.0	678029	99264	270319	0.00	6.71	11.28	60.14	39.61
15	58	36	14.0	796869	147069	220632	10.80	6.72	11.39	60.05	39.04
16	8	40	24.1	801374	151920	214873	20.87	6.74	11.49	59.96	38.50
16	18	42	34.1	806641	153307	214068	30.90	6.75	11.58	59.90	38.00
16	28	46	44.2	805905	154119	212964	40.97	6.77	11.71	59.73	37.35
16	38	48	54.2	802986	154615	212166	51.00	6.78	11.79	59.72	36.91
16	48	52	64.3	803776	155492	211813	61.07	6.79	11.87	59.62	36.45
16	58	54	74.3	803777	156253	211484	71.10	6.80	11.95	59.55	36.03
17	8	58	84.4	803183	156655	210812	81.17	6.82	12.02	59.45	35.67
17	19	0	94.4	804483	157688	210252	91.20	6.85	12.13	59.28	35.07
17	29	4	104.5	806078	158497	209930	101.27	6.87	12.21	59.14	34.64
17	39	6	114.5	805986	158977	209191	111.30	6.90	12.29	59.00	34.21
17	49	10	124.6	806795	159536	208547	121.37	6.93	12.37	58.83	33.77

$t_{correct.}$	Partial pressure (kPa)		Rate (mmol L^{-1} h^{-1})		$d[H_2O_2]/dt$	$\Sigma[H_2]$	$[H_2O_2]$	S_e	$\Sigma_2/[H_2O_2]$	$\Sigma_1/[H_2O_2]$
(min)	p_{H2}	p_{O2}	r_{H2}	r_{O2}	(mmol L^{-1} h^{-1})	(mmol L^{-1})	(mmol L^{-1})	(—)	(h)	(—)
0.00	17.19	28.92	90.32	66.08	41.84	0.00	0.00		0.000	0.000
10.80	17.17	29.10	90.18	65.12	40.06	16.25	7.37	0.45	0.090	2.204
20.87	17.16	29.27	90.05	64.23	38.40	31.37	13.96	0.44	0.176	2.248
30.90	17.14	29.43	89.96	63.39	36.81	46.42	20.24	0.44	0.262	2.293
40.97	17.15	29.62	89.71	62.30	34.89	61.50	26.26	0.43	0.351	2.342
51.00	17.11	29.77	89.70	61.57	33.44	76.50	31.97	0.42	0.440	2.393
61.07	17.11	29.91	89.54	60.79	32.05	91.53	37.46	0.41	0.531	2.443
71.10	17.10	30.03	89.44	60.11	30.78	106.50	42.72	0.40	0.623	2.493
81.17	17.10	30.14	89.30	59.49	29.69	121.49	47.79	0.39	0.716	2.542
91.20	17.11	30.31	89.03	58.50	27.96	136.40	52.61	0.39	0.810	2.593
101.27	17.13	30.43	88.82	57.78	26.73	151.32	57.20	0.38	0.906	2.645
111.30	17.14	30.55	88.61	57.06	25.51	166.16	61.57	0.37	1.003	2.699
121.37	17.16	30.66	88.36	56.33	24.31	181.00	65.75	0.36	1.102	2.753

H_2O_2 Synthesis Data Sheet

Entry No. 66 (Exp. Y163) Employed in: Fig. 10 Fig. 11

Catalyst, Additives			Reaction conditions		Gas feed rate (sccm)				
Name	Conc.	(Unit)	T_0 (℃)	18.4		H_2	O_2	N_2	Sum
Pd-PVP	8.33	(mg/L)	T (℃)	29.8	Set	17.00	20.00	20.00	57.00
$IrCl_3$	0.1734	(mg-Ir/L)	P_0 (hPa)	1016.2	Calibrated	16.90	18.70	19.99	55.59
H_2SO_4	0.01	(N)	P (hPa)	1022.8	Determination of final $[H_2O_2]$		Sample (g)	Absorbance (—)	$[H_2O_2]$ (mmol L^{-1})
NaBr	0.001	(N)	Agitation (rpm)	1203					
							0.415	0.738	59.94
Comment: Catalyst activation: H_2 gas 20 sccm at 303 K for 40 min.					Analysis of H_2O_2 formation selectivity and H_2O_2 destruction rate			S_f (—)	0.4559
								k_d[Cat] (h^{-1})	0.2751
								R^2	0.9994

GC calibration		GC count			Ratio of sensitivity (toward N_2)				Feed gas measurement	
Timing	No.	H_2	O_2	N_2	H_2		O_2			
Before reaction	1	1457216	178464	155191	0.0900	0.0899	0.813	0.813	T_a (℃)	17.6
	2	1455670	178382	155088	0.0900		0.813		P_0 (hPa)	1016.8
	3	1454517	178056	154893	0.0900		0.814		Flow	(cc/min)
After reaction	4	1450113	177199	153891	0.0897		0.812		H_2	18.28
	5	1449048	177301	154017	0.0898		0.812		O_2	20.23
	6	1449486	177339	154030	0.0898		0.812		N_2	21.63

Time				GC count			$t_{correct.}$	Outlet flow (sccm)		Conversion(%)	
H	M	S	min.	H_2	O_2	N_2	(min)	H_2	O_2	H_2	O_2
12	0	34	4.0	728296	101308	276259	0.00	6.49	11.14	61.61	40.43
12	10	36	14.0	838346	148852	226930	11.42	6.51	11.26	61.46	39.77
12	20	40	24.1	817748	155466	223371	21.49	6.53	11.37	61.33	39.20
12	30	42	34.1	811726	157069	222371	31.52	6.56	11.48	61.17	38.61
12	40	46	44.2	809834	157945	221534	41.59	6.57	11.59	61.12	38.04
12	50	48	54.2	810718	158791	220585	51.62	6.61	11.70	60.91	37.44
13	0	52	64.3	810853	159548	219619	61.69	6.64	11.81	60.73	36.86
13	10	54	74.3	812139	160267	218567	71.72	6.68	11.92	60.48	36.27
13	20	58	84.4	813887	161239	217706	81.79	6.72	12.04	60.23	35.63
13	31	0	94.4	817037	162043	216648	91.82	6.78	12.16	59.89	34.99
13	41	2	104.5	818773	162786	215773	101.86	6.82	12.26	59.64	34.43
13	51	6	114.5	822911	163608	214865	111.92	6.88	12.37	59.26	33.82
14	1	8	124.6	824293	164251	213923	121.96	6.93	12.48	59.01	33.27

$t_{correct.}$	Partial pressure (kPa)		Rate (mmol L^{-1} h^{-1})		$d[H_2O_2]/dt$	$\Sigma[H_2]$	$[H_2O_2]$	S_e	$\Sigma_2/[H_2O_2]$	$\Sigma_1/[H_2O_2]$
(min)	p_{H2}	p_{O2}	r_{H2}	r_{O2}	(mmol L^{-1} h^{-1})	(mmol L^{-1})	(mmol L^{-1})	(—)	(h)	(—)
0.00	16.90	29.02	92.94	67.49	42.05	0.00	0.00		0.000	0.000
11.42	16.90	29.22	92.72	66.41	40.09	17.67	7.82	0.44	0.095	2.260
21.49	16.90	29.40	92.52	65.44	38.36	33.21	14.40	0.43	0.181	2.306
31.52	16.91	29.58	92.29	64.46	36.64	48.67	20.67	0.42	0.268	2.354
41.59	16.88	29.77	92.20	63.50	34.81	64.14	26.67	0.42	0.357	2.405
51.62	16.91	29.94	91.88	62.50	33.12	79.53	32.34	0.41	0.447	2.459
61.69	16.92	30.11	91.62	61.54	31.47	94.93	37.76	0.40	0.538	2.514
71.72	16.96	30.27	91.24	60.56	29.88	110.22	42.89	0.39	0.631	2.570
81.79	17.00	30.45	90.87	59.49	28.11	125.49	47.76	0.38	0.726	2.628
91.82	17.07	30.61	90.34	58.43	26.51	140.64	52.32	0.37	0.823	2.688
101.86	17.11	30.76	89.97	57.49	25.00	155.72	56.63	0.36	0.921	2.750
111.92	17.19	30.91	89.40	56.47	23.53	170.77	60.70	0.36	1.021	2.813
121.96	17.23	31.05	89.03	55.55	22.06	185.69	64.51	0.35	1.123	2.878

S2. Original CASTEP data; Energy level of H on the first layer of M-Pd(111)

DFT studies were preliminarily performed to elucidate the great addition effects of Pt or Ir to the Pd-PVP colloid catalyst and the little effects of Ru, Rh and Au. First-principles quantum mechanics calculations were carried out with supercell models using CASTEP [1], which employs the density functional theory plane-wave pseudopotential method. GGA-PBE functional [2] was used with ultrasoft pseudopotentials [3]. The energy cutoff and Monkhorst-Pack mesh of k points were 400 eV and (4×4×1), respectively for all the models. A vacuum space with a height of 20 Å was placed over the surface of each supercell model.

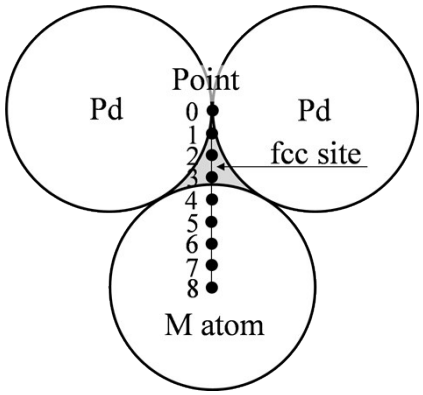

Fig. S1. Schematic overview of points over which H atom was located.

Adsorption energies of H were calculated using the models formed by replacing the central surface Pd atom of the Pd (111) 3×3×3 supercell with an M atom (M = Pt, Ir, Ru, Rh and Au) as shown in Fig. S1. These supercell slabs were geometrically optimized by fixing the third layer and in spin-polarized condition applying the formal spin as initial. Table S1 shows the coordinates of the geometrically optimized structures.

The energy level of a H atom located on the surface of a supercell slab was determined by Eq. (S1), in which ΔE_H, $E[Slab_1]$, $E[Slab_0]$, and $E[H_2]$ represent the energy level of the H atom, the energies of the H-bearing slab, the mother slab, and H_2, respectively. Here, calculation of $[Slab_1]$ and $[Slab_0]$ was performed in non-spin-polarized mode, because it was confirmed that the state of spin should be ignored for determining ΔE_H by Eq. (1) in separated calculations.

$$\Delta E_H = E[Slab_1] - E[Slab_0] - E[H_2]/2 \qquad \text{(S1)}$$

The adsorption energy profiles of H were determined right above the line segment connecting the center of the M atom and the point of contact of the adjacent two Pd atoms through the fcc hollow site. Points 0 to 8 were defined at equal intervals on the line segment, and H was vertically placed over each point by varying the height, *h* (0.1 Å intervals). Single-point energy calculation of $E[Slab_0]$ and $E[Slab_1]$ was carried out, and ΔE_H was determined according to Eq. (S1) at each height. The adsorption energy of H at each point, ΔE_{ad}, was determined as the minimum value of ΔE_H by applying a quadratic polynomial to the smallest 3 values of ΔE_H. Table S2 shows the coordinates of H atom and corresponding final energies.

References:

[1] Clark, S. J.; Segall, M. D.; Pickard, C. J.; Hasnip, P. J.; Probert, M. J.; Refson, K.; Payne, M. C. *Zeitschrift fuer Kristallographie* **2005**, 220, 567-570.
[2] Perdew, J. P.; Burke, K.; Ernzerhof, M. *Phys. Rev. Lett*. **1996**, 77, 3865-3868.
[3] Vanderbilt, D. *Phys. Rev. B* **1990**, 41, 7892-7895.

Table S1. Coordinates data for structure-optimized M-Pd(111) models.

(1) M = Pd

Atom	No.	Fractional coordinates of atoms			Lattice parameters	
		u	v	w		
Pd	1	-0.000252	0.000234	0.184082	a (angstrom)	8.3834
Pd	2	0.222166	0.111143	0.092070	b (angstrom)	8.3834
Pd	3	0.111111	0.222222	0.000000	c (angstrom)	24.5634
Pd	4	0.333108	0.000220	0.184090	Alpha (deg)	90.0000
Pd	5	0.555546	0.111121	0.092070	Beta (deg)	90.0000
Pd	6	0.444444	0.222222	0.000000	Gamma (deg)	120.0000
Pd	7	0.666459	0.000226	0.184075		
Pd	8	0.888840	0.111111	0.092069		
Pd	9	0.777778	0.222222	0.000000		
Pd	10	-0.000227	0.333540	0.184071		
Pd	11	0.222197	0.444472	0.092068		
Pd	12	0.111111	0.555556	0.000000		
Pd	13	0.333090	0.333572	0.184077		
Pd	14	0.555525	0.444499	0.092070		
Pd	15	0.444444	0.555556	0.000000		
Pd	16	0.666430	0.333547	0.184091		
Pd	17	0.888870	0.444457	0.092067		
Pd	18	0.777778	0.555556	0.000000		
Pd	19	-0.000224	0.666912	0.184094		
Pd	20	0.222211	0.777800	0.092071		
Pd	21	0.111111	0.888889	0.000000		
Pd	22	0.333113	0.666885	0.184076		
Pd	23	0.555546	0.777828	0.092070		
Pd	24	0.444444	0.888889	0.000000		
Pd	25	0.666430	0.666925	0.184078		
Pd	26	0.888841	0.777834	0.092071		
Pd	27	0.777778	0.888889	0.000000		

(2) M = Pt

Atom	No.	Fractional coordinates of atoms			Lattice parameters	
		u	v	w		
Pd	1	0.000456	0.000903	0.184679	a (angstrom)	8.3834
Pd	2	0.221241	0.108831	0.091436	b (angstrom)	8.3834
Pd	3	0.111111	0.222222	0.000000	c (angstrom)	24.5634
Pd	4	0.333385	0.000563	0.184939	Alpha (deg)	90.0000
Pd	5	0.554917	0.111843	0.092468	Beta (deg)	90.0000
Pd	6	0.444444	0.222222	0.000000	Gamma (deg)	120.0000
Pd	7	0.666687	-0.000037	0.184241		
Pd	8	0.888453	0.110843	0.092126		
Pd	9	0.777778	0.222222	0.000000		
Pd	10	0.000929	0.333462	0.184552		
Pd	11	0.220796	0.445874	0.091340		
Pd	12	0.111111	0.555556	0.000000		
Pd	13	0.557829	0.445390	0.091439		
Pd	14	0.444444	0.555556	0.000000		
Pd	15	0.666111	0.333356	0.184973		
Pd	16	0.888694	0.444139	0.092497		
Pd	17	0.777778	0.555556	0.000000		
Pd	18	-0.000257	0.667109	0.184098		

Pd	19	0.222480	0.777881	0.092512
Pd	20	0.111111	0.888889	0.000000
Pd	21	0.333278	0.665783	0.184591
Pd	22	0.555675	0.778217	0.092131
Pd	23	0.444444	0.888889	0.000000
Pd	24	0.665815	0.666308	0.184666
Pd	25	0.888720	0.778155	0.092515
Pd	26	0.777778	0.888889	0.000000
Pt	1	0.334642	0.332255	0.181243

(3) M = Ir

Atom	No.	Fractional coordinates of atoms			Lattice parameters	
		u	v	w		
Pd	1	0.003422	0.004083	0.185841	a (angstrom)	8.3834
Pd	2	0.220924	0.108502	0.093216	b (angstrom)	8.3834
Pd	3	0.111111	0.222222	0.000000	c (angstrom)	24.5634
Pd	4	0.333944	0.003719	0.185858	Alpha (deg)	90.0000
Pd	5	0.556372	0.110297	0.091712	Beta (deg)	90.0000
Pd	6	0.444444	0.222222	0.000000	Gamma (deg)	120.0000
Pd	7	0.666655	0.000011	0.184219		
Pd	8	0.887364	0.110302	0.091698		
Pd	9	0.777778	0.222222	0.000000		
Pd	10	0.003035	0.332621	0.185767		
Pd	11	0.220708	0.445956	0.093148		
Pd	12	0.111111	0.555556	0.000000		
Pd	13	0.558165	0.445743	0.093217		
Pd	14	0.444444	0.555556	0.000000		
Pd	15	0.662948	0.332723	0.185857		
Pd	16	0.888673	0.444239	0.092756		
Pd	17	0.777778	0.555556	0.000000		
Pd	18	-0.000172	0.666838	0.185046		
Pd	19	0.222426	0.777992	0.092756		
Pd	20	0.111111	0.888889	0.000000		
Pd	21	0.334046	0.663633	0.185768		
Pd	22	0.556367	0.779305	0.091698		
Pd	23	0.444444	0.888889	0.000000		
Pd	24	0.662584	0.663245	0.185841		
Pd	25	0.888608	0.778059	0.092673		
Pd	26	0.777778	0.888889	0.000000		
Ir	1	0.333122	0.333545	0.179040		

(4) M = Ru

Atom	No.	Fractional coordinates of atoms			Lattice parameters	
		u	v	w		
Ru	1	0.331161	0.332388	0.174821	a (angstrom)	8.3834
Pd	1	0.006722	0.007171	0.184618	b (angstrom)	8.3834
Pd	2	0.221729	0.109877	0.090996	c (angstrom)	24.5634
Pd	3	0.111111	0.222222	0.000000	Alpha (deg)	90.0000
Pd	4	0.332729	0.006227	0.184561	Beta (deg)	90.0000
Pd	5	0.556370	0.110914	0.092705	Gamma (deg)	120.0000
Pd	6	0.444444	0.222222	0.000000		
Pd	7	0.666207	-0.000024	0.184910		
Pd	8	0.888126	0.110784	0.092478		

Pd	9	0.777778	0.222222	0.000000
Pd	10	0.006050	0.333740	0.184654
Pd	11	0.221473	0.445297	0.091078
Pd	12	0.111111	0.555556	0.000000
Pd	13	0.557357	0.445419	0.091977
Pd	14	0.444444	0.555556	0.000000
Pd	15	0.660820	0.333904	0.185144
Pd	16	0.888469	0.444738	0.093545
Pd	17	0.777778	0.555556	0.000000
Pd	18	-0.000565	0.666897	0.185306
Pd	19	0.222036	0.777835	0.093205
Pd	20	0.111111	0.888889	0.000000
Pd	21	0.332798	0.660688	0.184492
Pd	22	0.556104	0.778657	0.092451
Pd	23	0.444444	0.888889	0.000000
Pd	24	0.660352	0.660651	0.184901
Pd	25	0.888724	0.777364	0.093493
Pd	26	0.777778	0.888889	0.000000

(5) M = Rh

Atom	No.	Fractional coordinates of atoms			Lattice parameters	
		u	v	w		
Rh	1	0.333823	0.334114	0.179170	a (angstrom)	8.3834
Pd	1	0.000371	0.001837	0.184467	b (angstrom)	8.3834
Pd	2	0.218998	0.108325	0.091480	c (angstrom)	24.5634
Pd	3	0.111111	0.222222	0.000000	Alpha (deg)	90.0000
Pd	4	0.330840	0.000484	0.183599	Beta (deg)	90.0000
Pd	5	0.554980	0.110622	0.091674	Gamma (deg)	120.0000
Pd	6	0.444444	0.222222	0.000000		
Pd	7	0.665151	-0.000167	0.183648		
Pd	8	0.888775	0.110713	0.092122		
Pd	9	0.777778	0.222222	0.000000		
Pd	10	0.000291	0.333616	0.183889		
Pd	11	0.219699	0.445497	0.091308		
Pd	12	0.111111	0.555556	0.000000		
Pd	13	0.556237	0.444770	0.091499		
Pd	14	0.444444	0.555556	0.000000		
Pd	15	0.663442	0.332252	0.183954		
Pd	16	0.886877	0.443626	0.092048		
Pd	17	0.777778	0.555556	0.000000		
Pd	18	-0.001923	0.665961	0.183909		
Pd	19	0.221051	0.776932	0.092170		
Pd	20	0.111111	0.888889	0.000000		
Pd	21	0.331793	0.665520	0.184131		
Pd	22	0.554406	0.777398	0.091867		
Pd	23	0.444444	0.888889	0.000000		
Pd	24	0.662483	0.662931	0.183523		
Pd	25	0.888833	0.778617	0.092320		
Pd	26	0.777778	0.888889	0.000000		

(6) M = Au

Atom	No.	Fractional coordinates of atoms			Lattice parameters
		u	v	w	

Pd	1	-0.002338	-0.000919	0.184110	a (angstrom)	8.3834
Pd	2	0.222421	0.112035	0.092658	b (angstrom)	8.3834
Pd	3	0.111111	0.222222	0.000000	c (angstrom)	24.5634
Pd	4	0.334064	-0.001257	0.184076	Alpha (deg)	90.0000
Pd	5	0.555836	0.110843	0.092008	Beta (deg)	90.0000
Pd	6	0.444444	0.222222	0.000000	Gamma (deg)	120.0000
Pd	7	0.666556	0.000148	0.183901		
Pd	8	0.887998	0.110856	0.091972		
Pd	9	0.777778	0.222222	0.000000		
Pd	10	-0.002440	0.333081	0.184038		
Pd	11	0.222664	0.443966	0.092671		
Pd	12	0.111111	0.555556	0.000000		
Pd	13	0.554584	0.444197	0.092678		
Pd	14	0.444444	0.555556	0.000000		
Pd	15	0.667918	0.332566	0.184073		
Pd	16	0.889569	0.446311	0.091845		
Pd	17	0.777778	0.555556	0.000000		
Pd	18	-0.000505	0.667179	0.184269		
Pd	19	0.220370	0.777138	0.091833		
Pd	20	0.111111	0.888889	0.000000		
Pd	21	0.333573	0.669089	0.184037		
Pd	22	0.555846	0.778705	0.091970		
Pd	23	0.444444	0.888889	0.000000		
Pd	24	0.667600	0.669007	0.184102		
Pd	25	0.889811	0.776865	0.091943		
Pd	26	0.777778	0.888889	0.000000		
Au	1	0.332969	0.333671	0.190819		

Table S2. Coordinates of H atom and corresponding final energy.

(1) M = Pd

Model	Point	Height (Å)	Fractional coordinates of H atom			Final Energy (eV)	ΔE_H (kcal g-atom^{-1})
			u	v	w		
H2						-31.69234394	
Pd						-21553.607893	
Pd_L107	8	1.5	0.333095	0.333574	0.245144	-21569.494802	-0.94
Pd_L108	8	1.6	0.333095	0.333574	0.249215	-21569.529385	-1.74
Pd_L109	8	1.7	0.333095	0.333574	0.253286	-21569.423412	0.71
Pd_L216	7	1.4	0.353921	0.375239	0.241073	-21569.339118	2.65
Pd_L217	7	1.5	0.353921	0.375239	0.245144	-21569.528750	-1.72
Pd_L218	7	1.6	0.353921	0.375239	0.249215	-21569.516794	-1.45
Pd_L226	6	1.4	0.374760	0.416362	0.241073	-21569.545943	-2.12
Pd_L227	6	1.5	0.374760	0.416362	0.245144	-21569.557619	-2.39
Pd_L228	6	1.6	0.374760	0.416362	0.249215	-21569.456379	-0.05
Pd_L234	5	1.2	0.395600	0.458571	0.232930	-21569.598738	-3.34
Pd_L235	5	1.3	0.395600	0.458571	0.237002	-21569.661680	-4.79
Pd_L236	5	1.4	0.395600	0.458571	0.241073	-21569.616828	-3.75
Pd_L241	4	0.9	0.416425	0.500236	0.220717	-21569.751970	-6.87
Pd_L242	4	1.0	0.416425	0.500236	0.224788	-21569.843090	-8.97
Pd_L243	4	1.1	0.416425	0.500236	0.228859	-21569.857946	-9.31
Pd_L250	3	0.8	0.437265	0.541908	0.216646	-21570.057951	-13.93
Pd_L251	3	0.9	0.437265	0.541908	0.220717	-21570.058351	-13.93
Pd_L252	3	1.0	0.437265	0.541908	0.224788	-21570.019091	-13.03
Pd_L260	2	0.8	0.458105	0.583568	0.216646	-21570.028070	-13.24

Pd_L261	2	0.9	0.458105	0.583568	0.220717	-21570.040173	-13.52
Pd_L262	2	1.0	0.458105	0.583568	0.224788	-21570.010189	-12.82
Pd_L271	1	0.9	0.478930	0.625233	0.220717	-21569.947970	-11.39
Pd_L272	1	1.0	0.478930	0.625233	0.224788	-21569.961692	-11.71
Pd_L273	1	1.1	0.478930	0.625233	0.228859	-21569.923763	-10.83
Pd_L281	0	0.9	0.499770	0.666905	0.220717	-21569.892484	-10.11
Pd_L282	0	1.0	0.499770	0.666905	0.224788	-21569.928645	-10.94
Pd_L283	0	1.1	0.499770	0.666905	0.228859	-21569.907355	-10.45

(2) M = Pt

Model	Point	Height (Å)	Fractional coordinates of H atom			Final Energy (eV)	ΔE_H (kcal g-atom^{-1})
			u	v	w		
H2						-31.69234394	
PdPt						-21473.102582	
PdPt_H_L107	8	1.5	0.334638	0.332258	0.242310	-21489.409257	-10.62
PdPt_H_L108	8	1.6	0.334638	0.332258	0.246381	-21489.473002	-12.09
PdPt_H_L109	8	1.7	0.334638	0.332258	0.250452	-21489.370198	-9.72
PdPt_H_L216	7	1.4	0.355257	0.373975	0.238663	-21489.238145	-6.67
PdPt_H_L217	7	1.5	0.355257	0.373975	0.242734	-21489.449810	-11.55
PdPt_H_L218	7	1.6	0.355257	0.373975	0.246805	-21489.442288	-11.38
PdPt_H_L226	6	1.4	0.375862	0.415697	0.239086	-21489.428195	-11.06
PdPt_H_L227	6	1.5	0.375862	0.415697	0.243157	-21489.433538	-11.18
PdPt_H_L228	6	1.6	0.375862	0.415697	0.247228	-21489.316545	-8.48
PdPt_H_L234	5	1.2	0.396481	0.457425	0.231367	-21489.392752	-10.24
PdPt_H_L235	5	1.3	0.396481	0.457425	0.235438	-21489.455608	-11.69
PdPt_H_L236	5	1.4	0.396481	0.457425	0.239509	-21489.403335	-10.48
PdPt_H_L242	4	1.0	0.417100	0.499154	0.223648	-21489.494378	-12.58
PdPt_H_L243	4	1.1	0.417100	0.499154	0.227719	-21489.520101	-13.18
PdPt_H_L244	4	1.2	0.417100	0.499154	0.231791	-21489.474243	-12.12
PdPt_H_L250	3	0.8	0.437706	0.540876	0.215929	-21489.553495	-13.95
PdPt_H_L251	3	0.9	0.437706	0.540876	0.220001	-21489.571295	-14.36
PdPt_H_L252	3	1.0	0.437706	0.540876	0.224072	-21489.544976	-13.75
PdPt_H_L260	2	0.8	0.458325	0.582605	0.216353	-21489.447317	-11.50
PdPt_H_L261	2	0.9	0.458325	0.582605	0.220424	-21489.475067	-12.14
PdPt_H_L262	2	1.0	0.458325	0.582605	0.224495	-21489.458786	-11.76
PdPt_H_L271	1	0.9	0.478930	0.624315	0.220843	-21489.368999	-9.69
PdPt_H_L272	1	1.0	0.478930	0.624315	0.224914	-21489.394458	-10.28
PdPt_H_L273	1	1.1	0.478930	0.624315	0.228986	-21489.366454	-9.63
PdPt_H_L281	0	0.9	0.499549	0.666043	0.221267	-21489.337985	-8.98
PdPt_H_L282	0	1.0	0.499549	0.666043	0.225338	-21489.379326	-9.93
PdPt_H_L283	0	1.1	0.499549	0.666043	0.229409	-21489.361868	-9.53

(3) M = Ir

Model	Point	Height (Å)	Fractional coordinates of H atom			Final Energy (eV)	ΔE_H (kcal g-atom^{-1})
			u	v	w		
H2						-31.69234394	
PdIr						-21312.795238	
PdIr_L207	8	1.5	0.333123	0.333540	0.240108	-21329.267734	-14.44
PdIr_L208	8	1.6	0.333123	0.333540	0.244179	-21329.380021	-17.03
PdIr_L209	8	1.7	0.333123	0.333540	0.248250	-21329.313656	-15.50
PdIr_L217	7	1.5	0.353769	0.374782	0.240951	-21329.342808	-16.17
PdIr_L218	7	1.6	0.353769	0.374782	0.245022	-21329.360682	-16.59

PdIr_L219	7	1.7	0.353769	0.374782	0.249093	-21329.239460	-13.79
PdIr_L226	6	1.4	0.374416	0.416011	0.237726	-21329.317887	-15.60
PdIr_L227	6	1.5	0.374416	0.416011	0.241797	-21329.337949	-16.06
PdIr_L228	6	1.6	0.374416	0.416011	0.245868	-21329.233105	-13.64
PdIr_L234	5	1.2	0.395063	0.457253	0.230431	-21329.246764	-13.96
PdIr_L235	5	1.3	0.395063	0.457253	0.234502	-21329.324548	-15.75
PdIr_L236	5	1.4	0.395063	0.457253	0.238573	-21329.284711	-14.83
PdIr_L242	4	1.0	0.415723	0.498489	0.223135	-21329.280642	-14.74
PdIr_L243	4	1.1	0.415723	0.498489	0.227206	-21329.329986	-15.88
PdIr_L244	4	1.2	0.415723	0.498489	0.231278	-21329.302699	-15.25
PdIr_L250	3	0.8	0.436370	0.539731	0.215836	-21329.259425	-14.25
PdIr_L251	3	0.9	0.436370	0.539731	0.219907	-21329.304849	-15.30
PdIr_L252	3	1.0	0.436370	0.539731	0.223978	-21329.302287	-15.24
PdIr_L261	2	0.9	0.457016	0.580960	0.220754	-21329.175776	-12.32
PdIr_L262	2	1.0	0.457016	0.580960	0.224825	-21329.181910	-12.46
PdIr_L263	2	1.1	0.457016	0.580960	0.228896	-21329.141732	-11.54
PdIr_L271	1	0.9	0.477663	0.622202	0.221601	-21329.047662	-9.37
PdIr_L272	1	1.0	0.477663	0.622202	0.225672	-21329.095237	-10.47
PdIr_L273	1	1.1	0.477663	0.622202	0.229743	-21329.085031	-10.23
PdIr_L281	0	0.9	0.498310	0.663432	0.222443	-21329.020003	-8.73
PdIr_L282	0	1.0	0.498310	0.663432	0.226514	-21329.077796	-10.06
PdIr_L283	0	1.1	0.498310	0.663432	0.230585	-21329.072771	-9.95

(4) M = Ru

Model	Point	Height (Å)	Fractional coordinates of H atom			Final Energy (eV)	ΔE_H (kcal g-atom^{-1})
			u	v	w		
H2						-31.69234394	
PdRu						-23356.234642	
PdRu_L207	8	1.5	0.331167	0.332395	0.235886	-23372.382579	-6.96
PdRu_L208	8	1.6	0.331167	0.332395	0.239957	-23372.479611	-9.20
PdRu_L209	8	1.7	0.331167	0.332395	0.244028	-23372.428989	-8.03
PdRu_L217	7	1.5	0.351841	0.373424	0.237124	-23372.458211	-8.70
PdRu_L218	7	1.6	0.351841	0.373424	0.241195	-23372.466060	-8.88
PdRu_L219	7	1.7	0.351841	0.373424	0.245266	-23372.362726	-6.50
PdRu_L226	6	1.4	0.372515	0.414453	0.234286	-23372.461658	-8.78
PdRu_L227	6	1.5	0.372515	0.414453	0.238357	-23372.464351	-8.84
PdRu_L228	6	1.6	0.372515	0.414453	0.242428	-23372.369422	-6.66
PdRu_L234	5	1.2	0.393189	0.455493	0.227377	-23372.455862	-8.65
PdRu_L235	5	1.3	0.393189	0.455493	0.231449	-23372.502757	-9.73
PdRu_L236	5	1.4	0.393189	0.455493	0.235520	-23372.458156	-8.70
PdRu_L242	4	1.0	0.413864	0.496522	0.220469	-23372.550065	-10.82
PdRu_L243	4	1.1	0.413864	0.496522	0.224540	-23372.582275	-11.56
PdRu_L244	4	1.2	0.413864	0.496522	0.228611	-23372.551454	-10.85
PdRu_L250	3	0.8	0.434552	0.537569	0.213560	-23372.608181	-12.16
PdRu_L251	3	0.9	0.434552	0.537569	0.217631	-23372.651388	-13.16
PdRu_L252	3	1.0	0.434552	0.537569	0.221702	-23372.651627	-13.16
PdRu_L260	2	0.8	0.455226	0.578598	0.214798	-23372.538927	-10.56
PdRu_L261	2	0.9	0.455226	0.578598	0.218869	-23372.601361	-12.00
PdRu_L262	2	1.0	0.455226	0.578598	0.222940	-23372.617335	-12.37
PdRu_L271	1	0.9	0.475900	0.619639	0.220102	-23372.505069	-9.78
PdRu_L272	1	1.0	0.475900	0.619639	0.224173	-23372.562557	-11.11
PdRu_L273	1	1.1	0.475900	0.619639	0.228245	-23372.561236	-11.08
PdRu_L282	0	1.0	0.496574	0.660667	0.225407	-23372.546704	-10.74

PdRu_L283	0	1.1	0.496574	0.660667	0.229478	-23372.546929	-10.75
PdRu_L284	0	1.2	0.496574	0.660667	0.233549	-23372.490737	-9.45

(5) M = Rh

Model	Point	Height (Å)	Fractional coordinates of H atom			Final Energy (eV)	ΔE_H (kcal g-atom^{-1})
			u	v	w		
H2						-31.69234394	
PdRh						-21361.328737	
PdRh_L207	8	1.5	0.333825	0.334118	0.240238	-21377.419080	-5.63
PdRh_L208	8	1.6	0.333825	0.334118	0.244309	-21377.476722	-6.96
PdRh_L209	8	1.7	0.333825	0.334118	0.248380	-21377.392813	-5.02
PdRh_L217	7	1.5	0.354238	0.375374	0.240820	-21377.470201	-6.81
PdRh_L218	7	1.6	0.354238	0.375374	0.244891	-21377.462029	-6.62
PdRh_L219	7	1.7	0.354238	0.375374	0.248962	-21377.342375	-3.86
PdRh_L226	6	1.4	0.374650	0.416641	0.237331	-21377.485618	-7.16
PdRh_L227	6	1.5	0.374650	0.416641	0.241402	-21377.485784	-7.17
PdRh_L228	6	1.6	0.374650	0.416641	0.245474	-21377.382941	-4.80
PdRh_L234	5	1.2	0.395063	0.457909	0.229771	-21377.507788	-7.68
PdRh_L235	5	1.3	0.395063	0.457909	0.233842	-21377.556185	-8.79
PdRh_L236	5	1.4	0.395063	0.457909	0.237913	-21377.510039	-7.73
PdRh_L242	4	1.0	0.415475	0.499165	0.222211	-21377.657352	-11.13
PdRh_L243	4	1.1	0.415475	0.499165	0.226282	-21377.681975	-11.69
PdRh_L244	4	1.2	0.415475	0.499165	0.230353	-21377.641498	-10.76
PdRh_L250	3	0.8	0.435901	0.540439	0.214651	-21377.770414	-13.73
PdRh_L251	3	0.9	0.435901	0.540439	0.218722	-21377.793053	-14.25
PdRh_L252	3	1.0	0.435901	0.540439	0.222793	-21377.773393	-13.80
PdRh_L260	2	0.8	0.456314	0.581695	0.215233	-21377.711066	-12.36
PdRh_L261	2	0.9	0.456314	0.581695	0.219304	-21377.744309	-13.13
PdRh_L262	2	1.0	0.456314	0.581695	0.223376	-21377.733663	-12.88
PdRh_L271	1	0.9	0.476726	0.622962	0.219887	-21377.644309	-10.82
PdRh_L272	1	1.0	0.476726	0.622962	0.223958	-21377.673955	-11.51
PdRh_L273	1	1.1	0.476726	0.622962	0.228029	-21377.649753	-10.95
PdRh_L281	0	0.9	0.497139	0.664230	0.220469	-21377.601625	-9.84
PdRh_L282	0	1.0	0.497139	0.664230	0.224540	-21377.645715	-10.86
PdRh_L283	0	1.1	0.497139	0.664230	0.228611	-21377.630721	-10.51

(6) M = Au

Model	Point	Height (Å)	Fractional coordinates of H atom			Final Energy (eV)	ΔE_H (kcal g-atom^{-1})
			u	v	w		
H2						-31.69234394	
PdAu						-21669.294232	
PdAu_L207	8	1.5	0.332971	0.333667	0.251886	-21684.825959	7.25
PdAu_L208	8	1.6	0.332971	0.333667	0.255957	-21684.915737	5.18
PdAu_L209	8	1.7	0.332971	0.333667	0.260028	-21684.842627	6.87
PdAu_L217	7	1.5	0.353921	0.375597	0.251043	-21684.842675	6.87
PdAu_L218	7	1.6	0.353921	0.375597	0.255114	-21684.915401	5.19
PdAu_L219	7	1.7	0.353921	0.375597	0.259185	-21684.837712	6.98
PdAu_L226	6	1.4	0.374870	0.417515	0.246129	-21684.798546	7.88
PdAu_L227	6	1.5	0.374870	0.417515	0.250200	-21684.925662	4.95
PdAu_L228	6	1.6	0.374870	0.417515	0.254271	-21684.897419	5.60
PdAu_L234	5	1.2	0.395820	0.459433	0.237140	-21684.743331	9.16
PdAu_L235	5	1.3	0.395820	0.459433	0.241211	-21684.945190	4.50

PdAu_L236	5	1.4	0.395820	0.459433	0.245282	-21684.998748	3.27
PdAu_L242	4	1.0	0.416784	0.501358	0.228155	-21685.061625	1.82
PdAu_L243	4	1.1	0.416784	0.501358	0.232226	-21685.162202	-0.50
PdAu_L244	4	1.2	0.416784	0.501358	0.236297	-21685.182905	-0.98
PdAu_L245	4	1.3	0.416784	0.501358	0.240368	-21685.136275	0.10
PdAu_L250	3	0.8	0.437733	0.543287	0.219170	-21685.438689	-6.88
PdAu_L251	3	0.9	0.437733	0.543287	0.223241	-21685.465739	-7.50
PdAu_L252	3	1.0	0.437733	0.543287	0.227312	-21685.451913	-7.18
PdAu_L260	2	0.8	0.458683	0.585205	0.218327	-21685.558931	-9.65
PdAu_L261	2	0.9	0.458683	0.585205	0.222398	-21685.570063	-9.91
PdAu_L262	2	1.0	0.458683	0.585205	0.226470	-21685.540107	-9.22
PdAu_L271	1	0.9	0.479633	0.627123	0.221552	-21685.547822	-9.40
PdAu_L272	1	1.0	0.479633	0.627123	0.225623	-21685.555205	-9.57
PdAu_L273	1	1.1	0.479633	0.627123	0.229694	-21685.512827	-8.59
PdAu_L281	0	0.9	0.500582	0.669041	0.220709	-21685.527281	-8.92
PdAu_L282	0	1.0	0.500582	0.669041	0.224780	-21685.562329	-9.73
PdAu_L283	0	1.1	0.500582	0.669041	0.228851	-21685.541076	-9.24