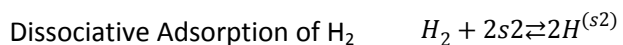


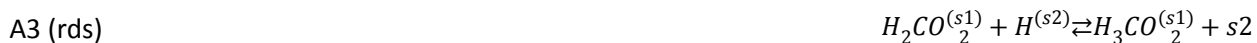
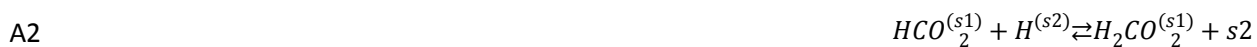
Kinetic model by Graaf¹

Mechanism:

Adsorption



CO₂-hydrogenation



rWGS



CO-hydrogenation



Rate equations:

$$r_{CO_2} = \frac{k_1 \cdot K_2 \left[f_{CO_2} \cdot f_{H_2}^{1,5} - \frac{f_{CH_3OH} \cdot f_{H_2O}}{f_{H_2}^{1,5}} \cdot \frac{1}{K_{eq,1}} \right]}{(1 + K_1 \cdot f_{CO} + K_2 \cdot f_{CO_2}) (f_{H_2}^{0,5} + K_3 \cdot f_{H_2O})}$$

$$r_{rWGS} = \frac{k_2 \cdot K_2 \left[f_{CO_2} \cdot f_{H_2} - f_{H_2O} \cdot f_{CO} \cdot \frac{1}{K_{eq,2}} \right]}{(1 + K_1 \cdot f_{CO} + K_2 \cdot f_{CO_2}) (f_{H_2}^{0,5} + K_3 \cdot f_{H_2O})}$$

$$r_{CO} = \frac{k_3 \cdot K_1 \left[f_{CO} \cdot f_{H_2}^{1,5} - \frac{f_{CH_3OH}}{f_{H_2}^{0,5}} \cdot \frac{1}{K_{eq,3}} \right]}{(1 + K_1 \cdot f_{CO} + K_2 \cdot f_{CO_2}) (f_{H_2}^{0,5} + K_3 \cdot f_{H_2O})}$$

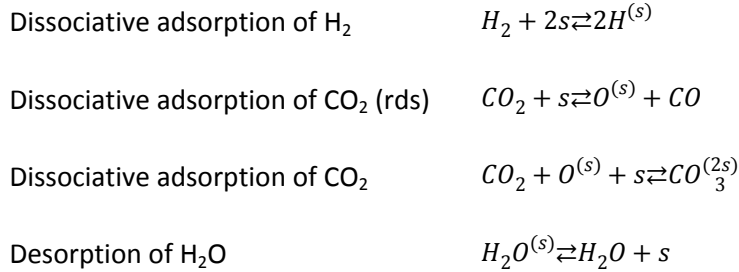
Original² and fitted kinetic parameters:

Parameter	Graaf _{original}	Graaf _{fit}	Unit
k_1	$1.09 \cdot 10^5 \cdot \exp\left(\frac{-87,500}{R \cdot T}\right)$	$5.861 \cdot 10^4 \cdot \exp\left(\frac{-62,403}{R \cdot T}\right)$	$mol \cdot kg_{cat}^{-1} \cdot s^{-1} \cdot bar^{-1}$
k_2	$9.64 \cdot 10^{11} \cdot \exp\left(\frac{-152,900}{R \cdot T}\right)$	$3.027 \cdot 10^{11} \cdot \exp\left(\frac{-123,083}{R \cdot T}\right)$	$mol \cdot kg_{cat}^{-1} \cdot s^{-1} \cdot bar^{-0,5}$
k_3	$4.89 \cdot 10^7 \cdot \exp\left(\frac{-113,000}{R \cdot T}\right)$	$-1.459 \cdot 10^8 \cdot \exp\left(\frac{-159,919}{R \cdot T}\right)$	$mol \cdot kg_{cat}^{-1} \cdot s^{-1} \cdot bar^{-1}$
K_1	$2.16 \cdot 10^{-5} \cdot \exp\left(\frac{46,800}{R \cdot T}\right)$	$6.830 \cdot 10^{-5} \cdot \exp\left(\frac{37,420}{R \cdot T}\right)$	bar^{-1}
K_2	$7.05 \cdot 10^{-7} \cdot \exp\left(\frac{61,700}{R \cdot T}\right)$	$8.014 \cdot 10^{-8} \cdot \exp\left(\frac{68,624}{R \cdot T}\right)$	bar^{-1}
K_3	$6.37 \cdot 10^{-9} \cdot \exp\left(\frac{84,000}{R \cdot T}\right)$	$1.181 \cdot 10^{-8} \cdot \exp\left(\frac{105,009}{R \cdot T}\right)$	$bar^{-0,5}$

Kinetic model by Bussche³

Mechanism:

Adsorption



CO₂-Hydrogenation



rWGS



Rate equations:

$$r_{CO_2} = \frac{k_{1,B} \cdot f_{CO_2} \cdot f_{H_2} \cdot \left[1 - \frac{f_{CH_3OH} \cdot f_{H_2O}}{f_{H_2}^3 \cdot f_{CO_2}} \cdot \frac{1}{K_{eq,1}} \right]}{\left(1 + K_{1,B} \cdot \left(\frac{f_{H_2O}}{f_{H_2}} \right) + K_{2,B} \cdot f_{H_2}^{0,5} + K_{3,B} \cdot f_{H_2O} \right)^3}$$

$$r_{rWGS} = \frac{k_{2,B} \cdot f_{CO_2} \cdot \left[1 - \frac{f_{CO} \cdot f_{H_2O}}{f_{CO_2} \cdot f_{H_2}} \cdot \frac{1}{K_{eq,2}} \right]}{\left(1 + K_{1,B} \left(\frac{f_{H_2O}}{f_{H_2}} \right) + K_{2,B} \cdot f_{H_2}^{0,5} + K_{3,B} \cdot f_{H_2O} \right)}$$

Original³ and fitted parameters:

Parameter	Bussche _{original}	Bussche _{fit}	Unit
$k_{1,B}$	$1.07 \cdot \exp\left(\frac{36,696}{R \cdot T}\right)$	$0.020 \cdot \exp\left(\frac{-29,122}{R \cdot T}\right)$	$mol \cdot kg_{cat}^{-1} \cdot s^{-1} \cdot bar^{-2}$
$k_{2,B}$	$1.22 \cdot 10^{10} \cdot \exp\left(\frac{-94,765}{R \cdot T}\right)$	$1.989 \cdot 10^9 \cdot \exp\left(\frac{-119,461}{R \cdot T}\right)$	$mol \cdot kg_{cat}^{-1} \cdot s^{-1} \cdot bar^{-1}$
$K_{1,B}$	3,453.38	$0.337 \cdot \exp\left(\frac{-2}{R \cdot T}\right)$	-
$K_{2,B}$	$0.499 \cdot \exp\left(\frac{17,197}{R \cdot T}\right)$	$-1.438 \cdot 10^{-3} \cdot \exp\left(\frac{17,263}{R \cdot T}\right)$	$bar^{-0,5}$
$K_{3,B}$	$6.62 \cdot 10^{-11} \cdot \exp\left(\frac{124,119}{R \cdot T}\right)$	$1.972 \cdot 10^{-10} \cdot \exp\left(\frac{90,516}{R \cdot T}\right)$	bar^{-1}

Kinetic model by Nestler⁴

Mechanism⁵:

Adsorption (see Graaf's model)

CO₂-hydrogenation (see Graaf's model)

rWGS (see Graaf's model)

Rate equations:

$$r_{CO_2} = \frac{k_1 \cdot K_2 \cdot f_{CO_2} \cdot f_{H_2}^{1,5} \cdot \left[1 - \frac{f_{CH_3OH} \cdot f_{H_2O}}{f_{H_2}^3 \cdot f_{CO_2}} \cdot \frac{1}{K_{eq,1}} \right]}{(1 + K_1 \cdot f_{CO} + K_2 \cdot f_{CO_2}) (f_{H_2}^{0,5} + K_3 \cdot f_{H_2O})}$$

$$r_{rWGS} = \frac{k_2 \cdot K_2 \cdot f_{CO_2} \cdot f_{H_2} \cdot \left[1 - \frac{f_{CO} \cdot f_{H_2O}}{f_{CO_2} \cdot f_{H_2}} \cdot \frac{1}{K_{eq,2}} \right]}{(1 + K_1 \cdot f_{CO} + K_2 \cdot f_{CO_2}) (f_{H_2}^{0,5} + K_3 \cdot f_{H_2O})}$$

Original⁴ and fitted parameters:

Parameter	Nestler _{original}	Nestler _{fit}	Unit
k_1	$5.411 \cdot 10^{-4} \cdot \exp\left(\frac{-45,458}{R \cdot T}\right)$	$2.385 \cdot 10^{-5} \cdot \exp\left(\frac{-14,709}{R \cdot T}\right)$	$mol \cdot kg_{cat}^{-1} \cdot s^{-1} \cdot Pa^{-1}$
k_2	$24.701 \cdot \exp\left(\frac{-54,970}{R \cdot T}\right)$	$244.433 \cdot \exp\left(\frac{-53,741}{R \cdot T}\right)$	$mol \cdot kg_{cat}^{-1} \cdot s^{-1} \cdot Pa^{-0,5}$
K_1	$3.321 \cdot 10^{-18} \cdot \exp\left(\frac{109,959}{R \cdot T}\right)$	$1.440 \cdot 10^{-17} \cdot \exp\left(\frac{-570}{R \cdot T}\right)$	Pa^{-1}
K_2	$8.262 \cdot 10^{-6}$	$4.223 \cdot 10^{-6}$	Pa^{-1}
K_3	$6.430 \cdot 10^{-14} \cdot \exp\left(\frac{119,570}{R \cdot T}\right)$	$6.407 \cdot 10^{-13} \cdot \exp\left(\frac{126,843}{R \cdot T}\right)$	$Pa^{-0,5}$

Miniplant experimental data

Point No	Feed composition			Reactor conditions			Product composition				Hot spot	
	COR	SN	GHSV	Ti01	Ti02	p	Y _{CO}	Y _{CO2}	Y _{MeOH}	Y _{H2O}	T _{Hotspot}	X _{Hotspot}
[-]	[-]	[-]	[h ⁻¹]	[°C]	[°C]	[bar]	[mol-%]	[mol-%]	[mol-%]	[mol-%]	[°C]	[m]
1	0.9	8	12,105	240.8	242.3	50	1.27%	5.73%	3.90%	4.36%	251.8	0.057
2	0.9	7	12,105	240.9	242.3	50	1.43%	6.74%	3.96%	4.44%	251.9	0.060
3	0.9	7	9,079	241.0	242.3	50	1.22%	6.54%	4.50%	4.78%	252.6	0.060
4	0.9	6	12,105	240.8	242.2	50	1.63%	7.98%	4.01%	4.59%	251.9	0.057
5	0.9	6	9,079	240.9	242.2	50	1.41%	7.86%	4.60%	4.94%	252.7	0.057
6	0.9	5	12,105	240.8	242.2	50	1.89%	9.69%	4.06%	4.68%	252.0	0.060
7	0.9	5	9,079	241.0	242.2	50	1.64%	9.52%	4.69%	5.03%	252.7	0.057
8	0.9	5	6,053	241.1	242.2	50	1.38%	9.32%	5.47%	5.53%	254.2	0.055
9	0.9	4	12,105	240.9	242.2	50	2.22%	11.94%	4.07%	4.76%	252.1	0.060
10	0.9	4	9,079	241.0	242.2	50	1.95%	11.98%	4.75%	5.14%	252.8	0.057
11	0.9	4	6,053	241.0	242.2	50	1.64%	11.81%	5.61%	5.65%	254.0	0.055
12	0.9	3	12,105	240.9	242.2	50	2.71%	15.42%	4.04%	4.81%	252.0	0.060
13	0.9	3	9,079	240.9	242.2	50	2.38%	15.38%	4.73%	5.15%	252.5	0.057
14	0.9	3	6,053	241.0	242.2	50	2.00%	15.25%	5.68%	5.71%	253.6	0.055
15	0.9	2	12,105	240.9	242.2	50	3.39%	20.35%	3.90%	4.75%	251.7	0.060
16	0.9	2	9,079	241.0	242.2	50	3.04%	20.58%	4.61%	5.08%	252.4	0.060
17	0.8	8	12,105	241.1	242.2	50	1.40%	5.39%	4.33%	3.79%	252.5	0.094
18	0.8	8	6,053	241.1	242.2	50	1.00%	5.00%	5.45%	4.47%	256.9	0.088
19	0.8	7	12,105	241.0	242.2	50	1.61%	6.33%	4.46%	3.87%	252.6	0.088
20	0.8	7	9,079	241.1	242.2	50	1.34%	6.23%	5.08%	4.22%	254.5	0.060
21	0.8	7	6,053	241.2	242.2	50	1.12%	5.86%	5.71%	4.57%	257.4	0.091
22	0.8	6	12,105	241.0	242.2	50	1.87%	7.51%	4.57%	3.92%	252.7	0.094
23	0.8	6	9,079	241.1	242.2	50	1.57%	7.41%	5.27%	4.29%	254.7	0.060
24	0.8	5	12,105	241.1	242.2	50	2.20%	9.02%	4.68%	3.96%	252.9	0.088
25	0.8	5	9,079	241.1	242.2	50	1.85%	9.00%	5.45%	4.36%	254.9	0.088
26	0.8	5	6,053	241.2	242.2	50	1.52%	8.77%	6.29%	4.82%	257.9	0.094
27	0.8	4	12,105	240.8	242.2	50	2.71%	11.39%	4.75%	3.98%	252.7	0.088
28	0.8	4	9,079	241.1	242.2	50	2.27%	11.35%	5.61%	4.35%	254.9	0.088
29	0.8	4	6,053	241.2	242.2	50	1.85%	11.19%	6.60%	4.87%	258.1	0.101
30	0.8	3	12,105	240.9	242.2	50	3.44%	14.58%	4.79%	3.93%	252.8	0.088
31	0.8	3	6,053	241.1	242.2	50	2.33%	14.49%	6.86%	4.83%	258.2	0.101
32	0.8	2	12,105	241.0	242.2	50	4.60%	19.59%	4.72%	3.72%	252.7	0.101
33	0.8	2	9,079	241.1	242.2	50	3.92%	19.87%	5.73%	4.07%	254.6	0.101
34	0.8	2	6,053	241.2	242.2	50	3.15%	20.01%	7.03%	4.53%	258.1	0.101
35	0.7	8	12,105	240.9	242.2	50	1.52%	4.94%	4.90%	3.30%	254.9	0.187
36	0.7	8	6,053	241.0	242.2	50	1.14%	3.98%	5.59%	3.35%	260.1	0.125
37	0.7	7	12,105	241.2	242.2	50	1.07%	4.65%	6.04%	3.91%	263.4	0.101

38	0.7	7	6,053	241.1	242.2	50	1.21%	5.46%	6.40%	4.00%	255.5	0.190
39	0.7	6	12,105	241.2	242.2	50	2.07%	6.90%	5.33%	3.42%	255.6	0.190
40	0.7	6	9,079	240.9	242.2	50	1.70%	6.80%	6.11%	3.73%	259.6	0.125
41	0.7	6	6,053	241.2	242.2	50	1.41%	6.59%	6.80%	4.12%	264.8	0.101
42	0.7	5	12,105	241.2	242.2	50	2.52%	8.39%	5.54%	3.41%	255.8	0.187
43	0.7	5	9,079	240.9	242.2	50	2.06%	8.35%	6.41%	3.75%	260.0	0.125
44	0.7	4	9,079	241.0	242.2	50	2.57%	10.52%	6.76%	3.71%	260.9	0.190
45	0.7	3	12,105	241.2	242.2	50	4.20%	13.63%	5.94%	3.23%	256.1	0.190
46	0.7	3	9,079	241.0	242.2	50	3.05%	12.22%	7.16%	3.56%	262.5	0.187
47	0.7	3	6,053	241.1	242.2	50	2.68%	13.80%	8.36%	3.94%	268.3	0.122
48	0.7	2	12,105	241.2	242.2	50	5.91%	18.52%	6.03%	2.95%	255.7	0.190
49	0.7	2	9,079	240.8	242.2	50	4.85%	18.93%	7.47%	3.25%	261.5	0.190
50	0.7	2	6,053	241.1	242.2	50	3.82%	19.24%	8.89%	3.53%	269.0	0.122
51	0.95	8	12,105	241.2	242.2	50	1.21%	5.99%	3.70%	4.63%	251.6	0.057
52	0.95	8	9,079	240.8	242.2	50	1.06%	5.78%	4.16%	4.93%	252.0	0.052
53	0.95	8	6,053	240.9	242.2	50	0.91%	5.52%	4.69%	5.33%	252.3	0.052
54	0.95	7	12,105	240.8	242.2	50	1.34%	6.91%	3.71%	4.77%	251.5	0.057
55	0.95	7	9,079	241.0	242.2	50	1.16%	6.69%	4.22%	5.08%	252.2	0.052
56	0.95	6	12,105	240.8	242.2	50	1.52%	8.20%	3.76%	4.92%	251.5	0.057
57	0.95	6	9,079	241.0	242.2	50	1.33%	8.06%	4.30%	5.27%	252.1	0.052
58	0.95	5	12,105	240.7	242.2	50	1.76%	9.96%	3.78%	5.07%	251.7	0.060
59	0.95	5	9,079	240.9	242.2	50	1.54%	9.89%	4.35%	5.43%	252.2	0.052
60	0.95	5	6,053	240.7	242.2	50	1.32%	9.60%	5.09%	5.90%	252.3	0.052
61	0.95	4	12,105	240.9	242.2	50	2.03%	12.25%	3.76%	5.17%	251.7	0.057
62	0.95	4	9,079	240.9	242.2	50	1.81%	12.15%	4.37%	5.56%	252.0	0.052
63	0.95	4	6,053	240.8	242.2	50	1.55%	12.03%	5.17%	6.08%	252.2	0.052
64	0.95	3	12,105	240.8	242.2	50	2.39%	15.73%	3.70%	5.29%	251.5	0.057
65	0.95	3	9,079	240.9	242.2	50	2.16%	15.60%	4.30%	5.64%	252.0	0.052
66	0.95	3	6,053	240.7	242.2	50	1.85%	15.54%	5.16%	6.17%	252.1	0.052
67	0.95	2	12,105	240.9	242.2	50	2.89%	20.70%	3.56%	5.34%	251.2	0.057
68	0.95	2	9,079	240.9	242.2	50	2.66%	20.84%	4.15%	5.71%	251.6	0.052
69	0.9	8	12,105	241.6	242.2	65	0.81%	4.99%	5.58%	5.55%	257.7	0.052
70	0.9	8	9,079	241.7	242.4	65	0.80%	4.93%	5.55%	5.58%	257.8	0.052
71	0.9	7	12,105	241.5	242.3	65	1.10%	6.25%	5.06%	5.28%	255.9	0.055
72	0.9	7	9,079	241.4	242.3	65	0.91%	5.91%	5.72%	5.74%	257.7	0.052
73	0.9	7	6,053	241.7	242.2	65	0.77%	5.67%	6.33%	5.85%	259.6	0.052
74	0.9	6	12,105	241.3	242.3	65	1.27%	7.42%	5.14%	5.42%	255.8	0.055
75	0.9	6	9,079	241.5	242.2	65	1.06%	7.19%	5.89%	5.91%	257.8	0.052
76	0.9	6	6,053	241.7	242.3	65	0.88%	6.92%	6.60%	6.09%	259.7	0.052
77	0.9	5	12,105	241.3	242.2	65	1.50%	9.11%	5.21%	5.53%	256.0	0.052
78	0.9	5	9,079	241.5	242.2	65	1.26%	8.91%	6.04%	6.10%	257.9	0.055
79	0.9	5	6,053	241.6	242.2	65	1.03%	8.62%	6.91%	6.38%	259.7	0.052

80	0.9	4	12,105	241.3	242.2	65	1.79%	11.49%	5.24%	5.60%	256.0	0.052
81	0.9	4	6,053	241.5	242.2	65	1.25%	11.14%	7.10%	6.35%	259.6	0.052
82	0.9	3	12,105	241.4	242.2	65	2.24%	15.12%	5.21%	5.62%	256.0	0.055
83	0.9	3	9,079	241.4	242.2	65	1.90%	15.02%	6.16%	6.17%	257.6	0.055
84	0.9	3	6,053	241.6	242.2	65	1.53%	14.49%	7.43%	6.92%	259.2	0.052
85	0.9	2	12,105	241.2	242.2	65	2.87%	20.22%	5.06%	5.50%	255.4	0.055
86	0.9	2	9,079	241.4	242.2	65	2.46%	20.35%	6.03%	6.00%	257.2	0.052
87	0.8	8	12,105	241.3	242.2	65	1.01%	4.82%	5.50%	4.65%	257.1	0.055
88	0.8	8	6,053	241.6	242.2	65	0.71%	4.30%	6.64%	5.41%	264.7	0.099
89	0.8	7	12,105	241.3	242.2	65	1.16%	5.73%	5.71%	4.73%	257.3	0.125
90	0.8	7	9,079	241.5	242.2	65	0.95%	5.47%	6.40%	5.19%	260.9	0.125
91	0.8	7	6,053	241.6	242.2	65	0.80%	5.20%	6.96%	5.40%	265.9	0.099
92	0.8	6	12,105	241.2	242.2	65	1.38%	6.97%	5.92%	4.80%	257.5	0.127
93	0.8	6	9,079	241.5	242.2	65	1.12%	6.71%	6.68%	5.31%	261.1	0.125
94	0.8	5	9,079	241.4	242.2	65	1.34%	8.32%	6.97%	5.37%	261.2	0.125
95	0.8	4	12,105	241.3	242.2	65	2.04%	10.99%	6.23%	4.90%	257.7	0.091
96	0.8	4	9,079	241.4	242.2	65	1.66%	10.79%	7.26%	5.45%	261.3	0.125
97	0.8	4	6,053	241.8	242.2	65	1.34%	10.54%	8.24%	5.67%	267.3	0.122
98	0.8	3	12,105	241.2	242.2	65	2.65%	14.19%	6.35%	4.78%	257.7	0.091
99	0.8	3	6,053	241.7	242.2	65	1.70%	14.02%	8.63%	5.57%	268.4	0.122
100	0.8	2	12,105	241.1	242.2	65	3.62%	19.59%	6.37%	4.56%	257.3	0.091
101	0.8	2	9,079	241.3	242.2	65	2.92%	19.73%	7.68%	4.97%	260.8	0.125
102	0.8	2	6,053	241.6	242.2	65	2.30%	19.78%	9.03%	5.48%	268.4	0.125
103	0.7	8	12,105	241.2	242.2	65	1.02%	4.34%	6.22%	4.22%	262.1	0.125
104	0.7	8	9,079	241.4	242.2	65	0.84%	4.12%	6.78%	4.50%	268.6	0.125
105	0.7	8	6,053	241.7	242.2	65	0.73%	3.95%	7.21%	4.80%	272.8	0.099
106	0.7	7	12,105	241.0	242.2	65	1.19%	5.21%	6.54%	4.25%	262.9	0.127
107	0.7	7	6,053	241.5	242.2	65	0.84%	4.78%	7.74%	4.85%	274.4	0.099
108	0.7	6	12,105	241.1	242.2	65	1.41%	6.38%	6.87%	4.33%	263.5	0.187
109	0.7	6	9,079	241.4	242.2	65	1.16%	6.11%	7.65%	4.67%	270.9	0.125
110	0.7	6	6,053	241.7	242.2	65	0.98%	5.88%	8.25%	5.00%	276.0	0.099
111	0.7	5	12,105	241.2	242.2	65	1.71%	7.85%	7.27%	4.30%	264.0	0.195
112	0.7	5	9,079	241.4	242.2	65	1.41%	7.71%	8.14%	4.69%	271.6	0.125
113	0.7	5	6,053	241.7	242.2	65	1.16%	7.49%	8.86%	5.15%	277.4	0.099
114	0.7	4	9,079	241.4	242.2	65	1.75%	10.00%	8.70%	4.79%	272.4	0.125
115	0.7	3	12,105	241.3	242.2	65	2.89%	13.46%	8.14%	4.10%	266.2	0.195
116	0.7	3	9,079	241.6	242.2	65	2.31%	13.35%	9.31%	4.60%	273.9	0.125
117	0.7	3	6,053	241.9	242.2	65	1.87%	13.21%	10.29%	4.97%	281.0	0.101
118	0.7	2	12,105	241.3	242.2	65	4.18%	18.74%	8.57%	3.78%	266.3	0.195
119	0.7	2	9,079	241.8	242.2	65	3.32%	18.95%	9.93%	4.18%	274.2	0.127
120	0.7	2	6,053	241.9	242.2	65	2.68%	19.12%	11.07%	4.54%	282.6	0.125
121	0.95	8	12,105	240.7	242.2	65	0.94%	5.44%	4.66%	5.36%	254.5	0.052

122	0.95	8	9,079	240.9	242.2	65	0.80%	5.17%	5.23%	5.79%	255.8	0.052
123	0.95	8	6,053	241.0	242.2	65	0.68%	4.91%	5.81%	5.98%	256.6	0.049
124	0.95	7	12,105	240.6	242.2	65	1.08%	6.43%	4.69%	5.54%	254.3	0.055
125	0.95	7	9,079	240.9	242.2	65	0.91%	6.19%	5.34%	5.96%	255.8	0.052
126	0.95	7	6,053	241.0	242.2	65	0.77%	5.90%	6.00%	6.13%	256.5	0.049
127	0.95	6	9,079	240.8	242.2	65	1.08%	7.58%	5.48%	6.17%	255.7	0.052
128	0.95	5	12,105	240.7	242.2	65	1.45%	9.56%	4.78%	5.82%	254.8	0.052
129	0.95	5	9,079	240.9	242.2	65	1.23%	9.20%	5.54%	6.37%	256.0	0.052
130	0.95	5	6,053	241.0	242.2	65	1.02%	8.85%	6.43%	6.68%	256.5	0.049
131	0.95	4	12,105	240.7	242.2	65	1.71%	11.86%	4.76%	5.93%	254.7	0.052
132	0.95	4	6,053	241.0	242.2	65	1.22%	11.43%	6.57%	6.91%	256.4	0.049
133	0.95	3	12,105	240.6	242.2	65	2.07%	15.35%	4.69%	6.01%	254.4	0.055
134	0.95	3	9,079	240.7	242.2	65	1.80%	15.20%	5.50%	6.46%	255.6	0.052
135	0.95	3	6,053	241.0	242.2	65	1.49%	15.12%	6.58%	6.89%	256.0	0.049
136	0.95	2	12,105	240.6	242.2	65	2.57%	20.52%	4.49%	6.03%	254.1	0.055
137	0.95	2	9,079	240.9	242.2	65	2.25%	20.46%	5.30%	6.53%	255.0	0.052
138	0.9	8	12,105	240.8	242.2	80	0.75%	4.76%	5.91%	5.90%	258.9	0.055
139	0.9	8	9,079	240.9	242.2	80	0.63%	4.41%	6.55%	6.32%	261.1	0.094
140	0.9	8	6,053	240.8	242.2	80	0.53%	4.12%	7.00%	6.25%	264.8	0.094
141	0.9	7	12,105	240.8	242.2	80	0.87%	5.65%	6.05%	6.09%	258.8	0.055
142	0.9	7	9,079	240.9	242.2	80	0.72%	5.33%	6.83%	6.72%	261.0	0.055
143	0.9	7	6,053	240.7	242.2	80	0.61%	4.94%	7.54%	6.94%	264.7	0.094
144	0.9	6	12,105	240.9	242.2	80	1.02%	7.01%	6.18%	6.25%	259.0	0.055
145	0.9	6	9,079	240.9	242.2	80	0.85%	6.62%	6.93%	6.49%	261.1	0.055
146	0.9	6	6,053	240.8	242.2	80	0.70%	6.23%	7.56%	6.48%	264.2	0.094
147	0.9	5	12,105	241.0	242.2	80	1.23%	8.66%	6.23%	6.44%	259.1	0.055
148	0.9	5	9,079	241.0	242.2	80	1.01%	8.22%	7.17%	7.06%	261.1	0.055
149	0.9	5	6,053	240.9	242.2	80	0.84%	7.99%	7.93%	6.58%	264.0	0.094
150	0.9	4	12,105	240.8	242.3	80	1.50%	11.07%	6.27%	6.44%	259.1	0.055
151	0.9	4	9,079	241.1	242.3	80	1.23%	10.80%	7.30%	7.03%	261.2	0.055
152	0.9	4	6,053	240.9	242.3	80	1.01%	10.30%	8.53%	7.77%	263.8	0.055
153	0.9	3	12,105	240.8	242.3	80	1.91%	14.50%	6.26%	6.37%	259.1	0.055
154	0.9	3	9,079	241.0	242.3	80	1.56%	14.24%	7.37%	6.84%	261.1	0.055
155	0.9	3	6,053	240.9	242.2	80	1.26%	14.01%	8.53%	7.32%	263.3	0.055
156	0.9	2	12,105	240.7	242.2	80	2.49%	19.97%	6.04%	6.21%	258.6	0.055
157	0.9	2	9,079	240.9	242.2	80	2.08%	19.96%	7.21%	6.82%	260.5	0.055
158	0.9	2	6,053	241.0	242.2	80	1.67%	19.93%	8.56%	7.14%	262.0	0.055
159	0.8	8	12,105	241.3	242.2	80	0.77%	4.30%	6.46%	5.38%	262.5	0.099
160	0.8	8	6,053	241.2	242.2	80	0.54%	3.74%	7.52%	5.77%	273.7	0.094
161	0.8	7	12,105	241.4	242.2	80	0.89%	5.18%	6.73%	5.50%	263.3	0.094
162	0.8	7	9,079	241.3	242.2	80	0.74%	4.87%	7.48%	5.85%	268.5	0.099
163	0.8	7	6,053	241.2	242.2	80	0.62%	4.60%	7.99%	5.99%	275.1	0.094

164	0.8	6	12,105	241.5	242.2	80	1.06%	6.46%	7.02%	5.66%	263.7	0.094
165	0.8	6	9,079	241.5	242.2	80	0.86%	6.06%	7.85%	6.05%	269.3	0.127
166	0.8	6	6,053	241.3	242.2	80	0.71%	5.68%	8.51%	6.46%	276.0	0.094
167	0.8	5	9,079	241.5	242.2	80	1.05%	7.74%	8.22%	6.18%	269.6	0.127
168	0.8	5	6,053	241.5	242.2	80	0.87%	7.41%	8.95%	6.26%	277.5	0.094
169	0.8	4	12,105	241.4	242.2	80	1.60%	10.44%	7.55%	5.76%	263.8	0.094
170	0.8	4	9,079	241.5	242.2	80	1.29%	10.10%	8.66%	6.33%	269.7	0.127
171	0.8	4	6,053	241.5	242.2	80	1.07%	9.77%	9.54%	6.77%	278.3	0.094
172	0.8	3	12,105	241.4	242.2	80	2.09%	13.68%	7.73%	5.61%	263.8	0.094
173	0.8	3	6,053	241.5	242.2	80	1.35%	13.31%	10.42%	7.13%	278.8	0.094
174	0.8	2	12,105	241.4	242.2	80	2.94%	19.30%	7.76%	5.19%	263.3	0.094
175	0.8	2	9,079	241.5	242.2	80	2.32%	19.34%	9.18%	5.85%	268.9	0.127
176	0.8	2	6,053	241.5	242.2	80	1.83%	19.06%	10.92%	7.19%	278.6	0.099
177	0.7	8	12,105	241.6	242.2	80	0.74%	3.81%	7.21%	4.93%	270.9	0.153
178	0.7	7	12,105	241.6	242.2	80	0.87%	4.65%	7.64%	4.98%	272.8	0.153
179	0.7	7	6,053	241.4	242.2	80	0.64%	4.12%	8.72%	5.52%	285.3	0.094
180	0.7	6	12,105	241.8	242.2	80	1.04%	5.77%	8.12%	5.08%	274.4	0.153
181	0.7	6	9,079	241.7	242.2	80	0.87%	5.52%	8.83%	5.49%	281.7	0.127
182	0.7	6	6,053	241.5	242.2	80	0.74%	5.19%	9.27%	5.58%	287.1	0.094
183	0.7	5	12,105	241.7	242.2	80	1.29%	7.31%	8.63%	5.20%	275.7	0.153
184	0.7	5	9,079	241.8	242.2	80	1.06%	7.07%	9.44%	5.65%	283.6	0.127
185	0.7	5	6,053	241.7	242.2	80	0.90%	6.72%	10.27%	6.17%	289.7	0.094
186	0.7	4	9,079	241.8	242.2	80	1.33%	9.23%	10.08%	5.67%	285.7	0.127
187	0.7	3	12,105	241.7	242.2	80	2.18%	12.95%	9.81%	5.04%	278.1	0.153
188	0.7	3	9,079	242.0	242.2	80	1.77%	12.84%	10.87%	5.58%	287.4	0.127
189	0.7	2	12,105	241.5	242.2	80	3.15%	18.55%	10.41%	4.57%	278.2	0.198
190	0.95	8	12,105	241.0	242.2	80	0.79%	5.01%	5.39%	5.97%	257.3	0.055
191	0.95	8	9,079	240.6	242.2	80	0.65%	4.68%	6.09%	6.51%	258.1	0.052
192	0.95	8	6,053	241.0	242.2	80	0.55%	4.31%	6.77%	6.84%	259.5	0.055
193	0.95	7	12,105	240.9	242.2	80	0.91%	6.07%	5.46%	6.20%	257.1	0.055
194	0.95	7	9,079	240.6	242.2	80	0.75%	5.64%	6.21%	6.51%	258.0	0.052
195	0.95	7	6,053	240.8	242.2	80	0.62%	5.24%	6.87%	6.48%	259.3	0.055
196	0.95	6	9,079	240.8	242.2	80	0.88%	6.95%	6.38%	6.98%	258.0	0.052
197	0.95	5	12,105	240.7	242.2	80	1.25%	9.01%	5.56%	6.49%	257.4	0.055
198	0.95	5	9,079	240.6	242.2	80	1.05%	8.72%	6.45%	6.95%	258.2	0.052
199	0.95	5	6,053	240.8	242.2	80	0.84%	8.23%	7.49%	7.45%	259.1	0.052
200	0.95	4	12,105	240.7	242.2	80	1.51%	11.51%	5.54%	6.61%	257.3	0.055
201	0.95	4	6,053	240.5	242.2	80	1.01%	10.72%	7.83%	8.01%	258.8	0.036
202	0.95	3	12,105	240.6	242.2	80	1.85%	15.10%	5.45%	6.72%	257.1	0.055
203	0.95	3	9,079	240.5	242.2	80	1.57%	14.71%	6.42%	7.07%	257.8	0.052
204	0.95	3	6,053	240.6	242.2	80	1.27%	14.40%	7.71%	7.62%	258.3	0.036
205	0.95	2	12,105	240.5	242.2	80	2.34%	20.18%	5.19%	6.55%	256.6	0.055

206	0.95	2	9,079	240.3	242.2	80	2.00%	20.20%	6.18%	7.12%	257.3	0.055
207	0.98	8	12,105	240.3	242.2	50	1.24%	6.21%	3.27%	4.63%	250.7	0.055
208	0.98	8	9,079	240.2	242.2	50	1.10%	6.08%	3.75%	4.92%	250.9	0.052
209	0.98	8	6,053	240.2	242.2	50	0.92%	5.70%	4.33%	5.36%	251.5	0.036
210	0.98	7	12,105	240.1	242.2	50	1.40%	7.20%	3.28%	4.77%	250.5	0.055
211	0.98	7	9,079	240.2	242.2	50	1.23%	7.02%	3.77%	5.10%	250.9	0.052
212	0.98	7	6,053	240.3	242.2	50	1.03%	6.71%	4.42%	5.55%	251.7	0.036
213	0.98	6	9,079	240.2	242.2	50	1.39%	8.32%	3.80%	5.24%	250.8	0.052
214	0.98	5	12,105	240.1	242.2	50	1.76%	10.19%	3.30%	5.08%	250.5	0.055
215	0.98	5	9,079	240.2	242.2	50	1.58%	10.10%	3.83%	5.40%	251.0	0.052
216	0.98	5	6,053	240.2	242.2	50	1.34%	9.88%	4.58%	5.95%	251.8	0.034
217	0.98	4	12,105	240.0	242.2	50	2.01%	12.59%	3.28%	5.25%	250.5	0.052
218	0.98	4	6,053	240.2	242.2	50	1.56%	12.14%	4.61%	6.12%	251.8	0.034
219	0.98	3	12,105	240.0	242.2	50	2.32%	15.97%	3.21%	5.42%	250.4	0.055
220	0.98	3	9,079	240.2	242.2	50	2.13%	15.90%	3.74%	5.74%	250.8	0.052
221	0.98	3	6,053	240.1	242.2	50	1.86%	15.80%	4.55%	6.29%	251.4	0.034
222	0.98	2	12,105	240.0	242.2	50	2.70%	21.04%	3.09%	5.53%	250.1	0.055
223	0.98	2	9,079	240.1	242.2	50	2.56%	20.97%	3.57%	5.88%	250.3	0.052
224	0.98	8	12,105	240.3	242.2	65	1.03%	5.75%	4.14%	5.26%	253.3	0.052
225	0.98	8	9,079	240.3	242.2	65	0.87%	5.51%	4.76%	5.73%	253.9	0.052
226	0.98	8	6,053	240.4	242.3	65	0.71%	5.12%	5.50%	6.33%	254.8	0.036
227	0.98	7	12,105	240.3	242.3	65	1.15%	6.83%	4.17%	5.41%	253.3	0.052
228	0.98	7	9,079	240.3	242.3	65	0.98%	6.53%	4.83%	5.90%	253.9	0.052
229	0.98	7	6,053	240.3	242.2	65	0.80%	6.15%	5.66%	6.54%	254.9	0.036
230	0.98	6	9,079	240.4	242.3	65	1.11%	7.77%	4.89%	6.07%	253.9	0.052
231	0.98	5	12,105	240.3	242.2	65	1.50%	9.89%	4.21%	5.75%	253.5	0.052
232	0.98	5	9,079	240.4	242.2	65	1.28%	9.46%	4.94%	6.26%	254.3	0.052
233	0.98	5	6,053	240.4	242.2	65	1.06%	9.09%	5.93%	7.01%	255.0	0.036
234	0.98	4	12,105	240.3	242.2	65	1.74%	12.10%	4.18%	5.90%	253.4	0.052
235	0.98	4	6,053	240.3	242.2	65	1.24%	11.62%	6.00%	7.19%	254.9	0.034
236	0.98	3	12,105	240.2	242.2	65	2.05%	15.62%	4.10%	6.07%	253.3	0.052
237	0.98	3	9,079	240.5	242.2	65	1.81%	15.45%	4.85%	6.57%	254.1	0.052
238	0.98	3	6,053	240.4	242.2	65	1.53%	15.23%	5.95%	7.32%	254.8	0.034
239	0.98	2	12,105	240.2	242.2	65	2.45%	20.42%	3.92%	6.16%	253.0	0.052
240	0.98	2	9,079	240.4	242.2	65	2.23%	20.73%	4.62%	6.65%	253.3	0.052
241	0.98	8	12,105	240.5	242.2	80	0.80%	5.18%	4.95%	6.05%	255.8	0.055
242	0.98	8	9,079	240.7	242.2	80	0.67%	4.86%	5.78%	6.57%	257.2	0.055
243	0.98	8	6,053	240.6	242.2	80	0.55%	4.44%	6.53%	6.86%	257.9	0.036
244	0.98	7	12,105	240.6	242.2	80	0.93%	6.25%	5.10%	6.15%	256.1	0.055
245	0.98	7	9,079	240.7	242.2	80	0.77%	5.86%	5.91%	6.76%	257.2	0.055
246	0.98	7	6,053	240.7	242.2	80	0.62%	5.41%	6.72%	6.84%	258.0	0.036
247	0.98	6	9,079	240.7	242.2	80	0.89%	7.11%	6.01%	6.99%	257.1	0.055

248	0.98	5	12,105	240.6	242.2	80	1.26%	9.29%	5.18%	6.52%	256.6	0.055
249	0.98	5	9,079	240.7	242.2	80	1.05%	8.96%	6.08%	7.07%	257.4	0.055
250	0.98	5	6,053	240.6	242.2	80	0.85%	8.44%	7.19%	7.63%	258.0	0.036
251	0.98	4	12,105	240.5	242.2	80	1.49%	11.67%	5.15%	6.66%	256.5	0.055
252	0.98	4	6,053	240.7	242.2	80	1.01%	10.96%	7.31%	7.82%	258.0	0.036
253	0.98	3	12,105	240.5	242.2	80	1.80%	15.20%	5.03%	6.79%	256.3	0.055
254	0.98	3	9,079	240.5	242.2	80	1.55%	14.85%	5.98%	7.40%	256.9	0.052
255	0.98	2	12,105	240.3	242.2	80	2.23%	20.59%	4.78%	6.82%	255.6	0.052
256	0.98	2	9,079	240.6	242.2	80	1.93%	20.40%	5.69%	7.46%	256.1	0.052
257	0.9	8	12,105	220.2	222.2	50	1.53%	6.75%	2.24%	2.99%	228.6	0.057
258	0.9	8	9,079	220.3	222.2	50	1.42%	6.53%	2.68%	3.31%	229.8	0.055
259	0.9	8	6,053	220.2	222.2	50	1.15%	6.19%	3.44%	3.82%	230.4	0.052
260	0.9	7	12,105	220.2	222.2	50	1.69%	7.81%	2.25%	3.06%	228.6	0.057
261	0.9	7	9,079	220.1	222.2	50	1.57%	7.49%	2.68%	3.39%	229.6	0.055
262	0.9	7	6,053	220.3	222.2	50	1.30%	7.31%	3.49%	3.90%	230.8	0.052
263	0.9	6	12,105	220.3	222.2	50	1.87%	9.07%	2.26%	3.10%	229.1	0.057
264	0.9	6	9,079	220.2	222.2	50	1.79%	8.86%	2.72%	3.47%	229.9	0.057
265	0.9	6	6,053	220.1	222.2	50	1.47%	8.47%	3.52%	3.96%	231.0	0.057
266	0.9	5	12,105	220.1	222.2	50	2.09%	10.78%	2.28%	3.15%	229.1	0.057
267	0.9	5	9,079	220.3	222.2	50	2.02%	10.54%	2.73%	3.52%	230.1	0.055
268	0.9	5	6,053	220.3	222.2	50	1.71%	10.35%	3.55%	4.04%	231.7	0.057
269	0.9	4	12,105	220.2	222.2	50	2.39%	13.00%	2.28%	3.19%	229.3	0.073
270	0.9	4	9,079	220.3	222.2	50	2.31%	12.74%	2.74%	3.56%	230.2	0.057
271	0.9	4	6,053	220.2	222.2	50	2.01%	12.55%	3.57%	4.09%	231.8	0.057
272	0.9	3	12,105	220.2	222.2	50	2.81%	16.44%	2.26%	3.22%	229.5	0.075
273	0.9	3	9,079	220.1	222.1	50	2.73%	16.32%	2.72%	3.60%	230.1	0.060
274	0.9	3	6,053	220.1	222.2	50	2.43%	16.13%	3.54%	4.09%	232.0	0.057
275	0.9	2	12,105	220.0	222.2	50	3.41%	21.28%	2.20%	3.20%	229.3	0.075
276	0.9	2	9,079	220.2	222.1	50	3.33%	21.36%	2.65%	3.56%	230.2	0.057
277	0.9	2	6,053	220.3	222.2	50	3.06%	21.47%	3.47%	4.06%	232.1	0.057
278	0.8	8	12,105	220.1	222.1	50	2.14%	6.29%	2.29%	2.54%	228.3	0.057
279	0.8	8	6,053	220.3	222.2	50	1.38%	5.81%	3.80%	3.26%	230.8	0.057
280	0.8	7	12,105	220.1	222.1	50	2.39%	7.19%	2.32%	2.59%	228.4	0.057
281	0.8	7	9,079	220.2	222.1	50	2.10%	7.03%	2.86%	2.84%	229.6	0.055
282	0.8	7	6,053	220.3	222.1	50	1.58%	6.79%	3.87%	3.30%	231.2	0.057
283	0.8	6	12,105	220.1	222.1	50	2.75%	8.44%	2.34%	2.59%	228.5	0.057
284	0.8	6	9,079	220.3	222.1	50	2.42%	8.17%	2.90%	2.86%	229.7	0.060
285	0.8	6	6,053	220.3	222.2	50	1.85%	8.00%	3.93%	3.32%	231.7	0.057
286	0.8	5	9,079	220.3	222.2	50	2.82%	9.85%	2.92%	2.89%	229.9	0.055
287	0.8	4	12,105	220.2	222.1	50	3.69%	12.12%	2.34%	2.63%	229.0	0.075
288	0.8	4	9,079	220.2	222.1	50	3.38%	11.94%	2.92%	2.88%	230.0	0.060
289	0.8	4	6,053	220.3	222.2	50	2.73%	11.95%	4.03%	3.31%	232.1	0.055

290	0.8	3	12,105	220.0	222.1	50	4.51%	15.30%	2.31%	2.60%	229.0	0.075
291	0.8	3	6,053	220.3	222.2	50	3.43%	15.25%	4.04%	3.23%	232.3	0.055
292	0.8	2	12,105	220.1	222.2	50	5.74%	19.79%	2.24%	2.47%	229.0	0.075
293	0.8	2	9,079	220.1	222.2	50	5.41%	20.05%	2.81%	2.73%	229.8	0.060
294	0.8	2	6,053	220.3	222.1	50	4.59%	20.18%	3.96%	3.08%	232.2	0.055
295	0.7	8	12,105	220.2	222.1	50	2.78%	5.74%	2.39%	2.14%	227.8	0.057
296	0.7	8	9,079	220.2	222.1	50	2.33%	5.47%	3.06%	2.37%	229.2	0.055
297	0.7	7	12,105	220.2	222.1	50	3.17%	6.57%	2.42%	2.16%	228.0	0.057
298	0.7	7	6,053	220.3	222.1	50	1.87%	6.23%	4.39%	2.83%	231.4	0.057
299	0.7	6	12,105	220.1	222.2	50	3.64%	7.51%	2.43%	2.16%	228.1	0.057
300	0.7	6	9,079	220.4	222.1	50	3.19%	7.48%	3.13%	2.35%	229.5	0.055
301	0.7	6	6,053	220.3	222.1	50	2.27%	7.41%	4.51%	2.80%	231.6	0.057
302	0.7	5	12,105	220.1	222.1	50	4.32%	8.97%	2.43%	2.17%	228.2	0.057
303	0.7	5	9,079	220.3	222.1	50	3.77%	8.94%	3.14%	2.33%	229.6	0.060
304	0.7	5	6,053	220.4	222.1	50	2.77%	8.92%	4.60%	2.76%	231.9	0.057
305	0.7	4	9,079	220.3	222.2	50	4.68%	11.00%	3.13%	2.33%	229.6	0.060
306	0.7	3	12,105	220.1	222.1	50	6.56%	13.70%	2.37%	2.09%	228.5	0.075
307	0.7	2	12,105	220.2	222.1	50	8.66%	18.26%	2.27%	1.98%	228.6	0.078
308	0.95	8	12,105	220.1	222.1	50	1.29%	7.01%	2.22%	3.28%	228.9	0.060
309	0.95	8	9,079	220.3	222.1	50	1.24%	6.81%	2.62%	3.64%	229.7	0.055
310	0.95	8	6,053	220.2	222.2	50	1.07%	6.48%	3.32%	4.15%	230.5	0.055
311	0.95	7	12,105	220.2	222.2	50	1.40%	8.05%	2.22%	3.33%	229.0	0.057
312	0.95	7	9,079	220.2	222.1	50	1.36%	7.77%	2.62%	3.72%	229.7	0.055
313	0.95	7	6,053	220.1	222.1	50	1.18%	7.41%	3.33%	4.24%	230.8	0.057
314	0.95	6	9,079	220.2	222.2	50	1.50%	9.09%	2.63%	3.80%	229.8	0.055
315	0.95	5	12,105	220.1	222.1	50	1.65%	11.14%	2.25%	3.47%	229.1	0.057
316	0.95	5	9,079	220.2	222.1	50	1.66%	10.86%	2.66%	3.89%	230.0	0.057
317	0.95	5	6,053	220.1	222.1	50	1.50%	10.57%	3.38%	4.45%	231.5	0.055
318	0.95	4	12,105	220.1	222.1	50	1.84%	13.43%	2.25%	3.53%	229.2	0.055
319	0.95	4	6,053	220.3	222.1	50	1.73%	12.95%	3.38%	4.56%	231.8	0.055
320	0.95	3	12,105	220.2	222.1	50	2.05%	16.88%	2.23%	3.58%	229.3	0.055
321	0.95	3	9,079	220.2	222.1	50	2.14%	16.56%	2.63%	4.04%	230.4	0.057
322	0.95	3	6,053	220.1	222.1	50	2.01%	16.46%	3.34%	4.63%	231.8	0.055
323	0.95	2	12,105	220.0	222.1	50	2.41%	22.07%	2.18%	3.57%	229.2	0.055
324	0.95	2	9,079	220.2	222.1	50	2.50%	21.77%	2.57%	4.04%	230.2	0.057

NMR liquid phase measurement

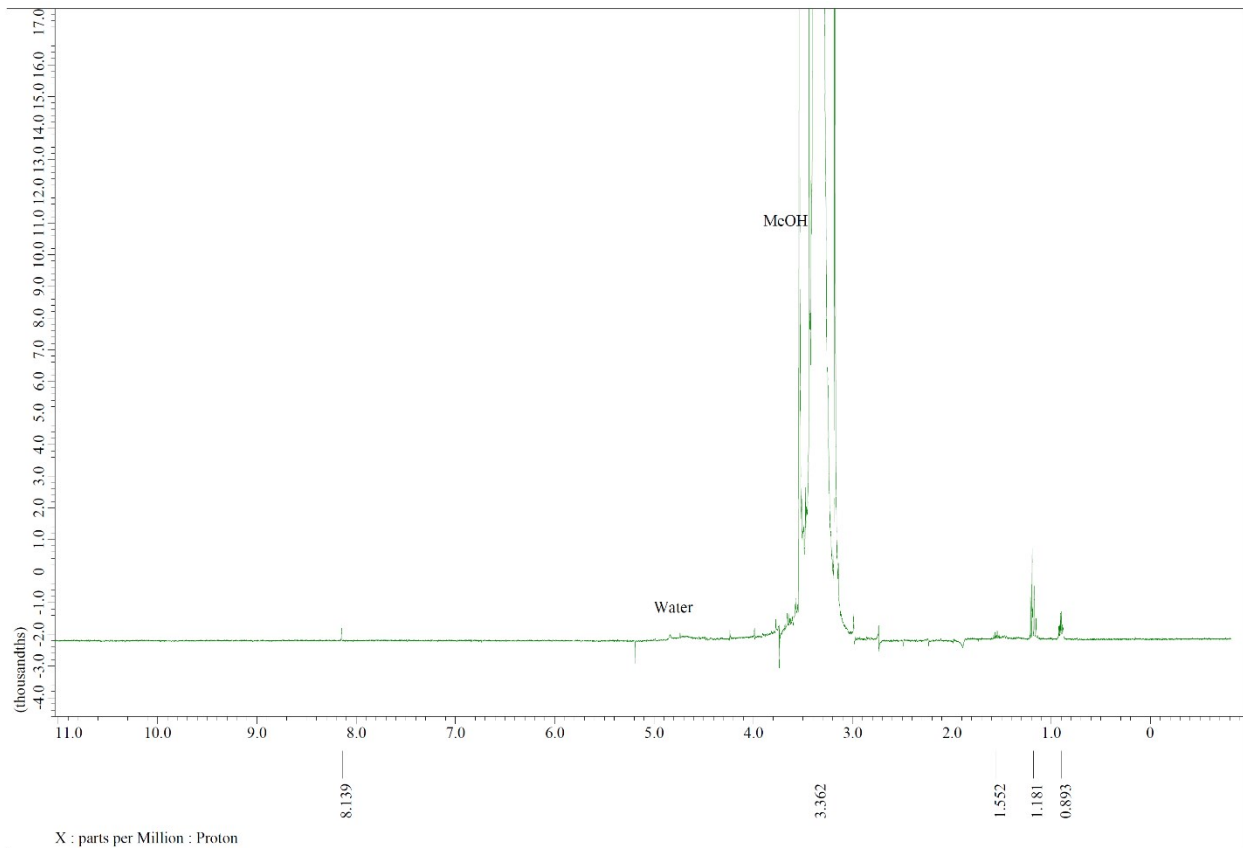


Figure 1: NMR measurement of a liquid phase sample; ^1H NMR (400 MHz, D_2O): $\delta/\text{ppm} = 8,139$ (s, HCOOH , traces), 4,8 (s, H_2O), 3,362 (s, CH_3OH ; $\text{CH}_3\text{CH}_2\text{OH}$ and $\text{CH}_3\text{CH}_2\text{CH}_2\text{OH}$ is covered by CH_3OH), 1,552 (m, $\text{CH}_3\text{CH}_2\text{CH}_2\text{OH}$), 1,181 (t, $\text{CH}_3\text{CH}_2\text{OH}$), 0,893 (t, $\text{CH}_3\text{CH}_2\text{CH}_2\text{OH}$).

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