Homogeneous and heterogeneous catalysis impact on pyrolyzed cellulose to produce bio-oil

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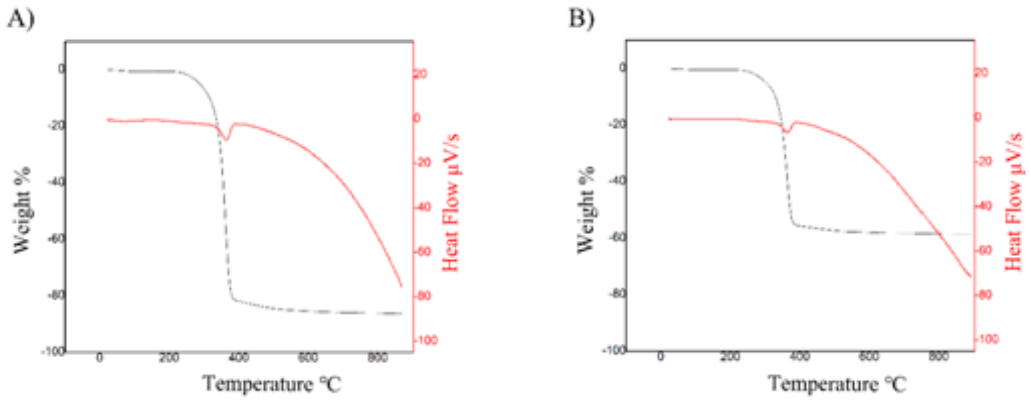

Figure S1.TG-DTA spectrum of a) cellulose b) cellulose with Ni_2Fe_3 catalyst

Table S1 Specific bio-oil compounds measured by GC-MS without catalyst

Compound name	Ret. Time (min)	Area percentage %
3-Penten-2-one, (E)-	8.1	1.9
2-Propanone, 1-hydroxy-	20.7	10.5
2-Cyclopenten-1-one	25.0	2.4
Acetic acid	33.2	3.6
Furfural	34.9	7.6
Propanoic acid, 2-oxo-, methyl ester	35.6	1.6
2-Propanone, 1-(acetyloxy)-	35.8	1.1
Ethanone, 1-(2-furanyl)-	37.4	0.6
2-Cyclopenten-1-one, 3-methyl-	37.6	0.5
Propanoic acid	40.1	1.8
2-Butanone, 1-(acetyloxy)-	40.3	1.5
2-Furancarboxaldehyde, 5-methyl-	42.1	4.8
Propanoic acid, 2-methyl-	42.3	0.5
Butyrolactone	44.6	0.7
Butanoic acid	46.0	1.1
2(5H)-Furanone, 5-methyl-	47.9	0.9
4-Methyl-2-oxo-(1H)-pyrimidine	48.8	1.4
2(5H)-Furanone	52.1	0.9
1,2-Cyclopentanedione	53.6	3.6
Crotonic acid	54.2	0.6
1,2-Cyclopentanedione, 3-methyl-	56.8	1.9
4-Methyl-5H-furan-2-one	59.1	0.5
Maltol	63.9	0.5
Phenol	67.2	0.5
Cyclopropyl carbinol	70.1	0.6
4-Methyl-2-oxopentanenitrile	75.9	0.8
Pentanoic acid, 4-oxo-	78.4	0.8
1,4:3,6-Dianhydro-.alpha.-d-glucopyranose	80.0	1.8
5-Hydroxymethylfurfural	82.6	1.0
.beta.-D-Glucopyranose, 1,6-anhydro-	98.354	44.0

Table S2 Specific bio-oil compounds measured by GC-MS with Ni_2Fe_3 catalyst

Compound name	Ret. Time (min)	Area percentage %
2-Butenal, (E)-	5.0	0.6
3-Penten-2-one, (E)-	8.4	1.6
2-Propanone, 1-hydroxy-	21.5	13.1
Acetic acid	33.4	3.1
2-Propanone, 1-methoxy-	34.3	7.3
Furfural	35.7	9.3
2-Butanone	35.8	0.4
Propanoic acid, 2-oxo-, methyl ester	36.4	1.7
2-Propanone, 1-(acetyloxy)-	36.6	1.1
Propanoic acid, ethyl ester	40.8	1.9
2-Butanone, 1-(acetyloxy)-	41.0	1.1
2-Furancarboxaldehyde, 5-methyl-	42.8	3.3
Butanoic acid	46.6	1.1
Methylpent-4-enylamine	47.4	0.5
2-Furanmethanol	48.7	4.0
4-Methyl-2-oxo-(1H)-pyrimidine	49.5	1.0
2(5H)-Furanone	52.8	0.5
1,2-Cyclopentanedione	54.3	5.1
Crotonic acid	54.8	0.5
2-Methylene cyclopentanol	56.0	0.4
1,2-Cyclopentanedione, 3-methyl-	57.4	2.5
4-Methyl-5H-furan-2-one	59.7	0.4
Phenol	68.0	0.6
Phenol, 2-methyl-	68.1	0.5
Cyclopropyl carbinol	70.8	1.5
Pentanoic acid, 4-oxo-	78.8	0.3
Decane, 5,6-dimethyl-	79.7	0.5
1,4:3,6-Dianhydro-.alpha.-d-glucopyranose	80.4	1.3
5-HydroxymethylFurfural	83.0	4.7
.beta.-D-Glucopyranose, 1,6-anhydro-	98.7	30.0

Table S3 Specific bio-oil compounds measured by GC-MS with ZSM-5 catalyst

Compound name	Ret. Time (min)	Area percentage %
2,3-Pentanedione	5.4	0.5
3-Penten-2-one, (E)-	8.1	0.8
2-Propanone, 1-hydroxy-	20.3	12.2
2-Cyclopenten-1-one	24.9	2.1
2-Cyclopenten-1-one, 2-methyl-	26.2	0.7
1-Hydroxy-2-butanone	27.2	0.6
Acetic acid	33.8	5.2
Furfural	34.9	9.4
2-Butanone	35.0	0.6
Propanoic acid, 2-oxo-, methyl ester	35.6	1.5
2-Propanone, 1-(acetyloxy)-	35.8	1.1
Ethanone, 1-(2-furanyl)-	37.4	1.0
Propanoic acid, ethenyl ester	40.1	0.5
Propanoic acid	40.3	2.1
2-Furancarboxaldehyde, 5-methyl-	42.1	4.0
Tetrazolo[1,5-b]pyridazine, 6-(1-piperidyl)-	44.6	0.8
Butanoic acid	46.0	1.0
2(5H)-Furanone, 5-methyl-	47.9	0.9
4-Methyl-2-oxo-(1H)-pyrimidine	48.8	1.4
2(5H)-Furanone	52.1	1.2
1,2-Cyclopentanedione	53.6	3.1
1,2-Cyclopentanedione, 3-methyl-	56.8	1.7
4-Methyl-5H-furan-2-one	59.1	0.7
Cyclopropyl carbinol	70.1	0.8
1,4-Dioxaspiro[2.4]heptan-5-one, 7-methyl-	72.3	0.7
4-Methyl-2-oxopentanenitrile	75.9	0.8
Pentanoic acid, 4-oxo-	78.4	0.8
1,4:3,6-Dianhydro-.alpha.-d-glucopyranose	79.9	0.8
5-Hydroxymethylfurfural	82.6	1.2
.beta.-D-Glucopyranose, 1,6-anhydro-	98.2	41.5

Table S4 Specific bio-oil compounds measured by GC-MS with Ni_2Fe_3/ZSM-5 catalyst

Compound name	Ret. Time (min)	Area percentage %
2,3-Pentanedione	5.4	0.6
3-Penten-2-one, (E)-	8.0	1.1
2-Propanone, 1-hydroxy-	20.2	13.4
2-Cyclopenten-1-one	24.8	1.7
2-Cyclopenten-1-one, 2-methyl-	26.2	0.7
1-Hydroxy-2-butanone	27.2	0.7
Acetic acid	33.9	5.6
Furfural	34.8	9.6
2-Butanone	35.0	1.1
Propanoic acid, 2-oxo-, methyl ester	35.5	2.4
2-Propanone, 1-(acetyloxy)-	35.8	1.1
Ethanone, 1-(2-furanyl)-	37.4	1.0
2-Butanone, 1-(acetyloxy)-	40.0	0.8
Propanoic acid	40.3	2.1
2-Furancarboxaldehyde, 5-methyl-	42.0	4.4
Butyrolactone	44.5	0.8
Butanoic acid	46.0	0.9
2(5H)-Furanone, 5-methyl-	47.9	1.1
4-Methyl-2-oxo-(1H)-pyrimidine	48.8	1.2
2(5H)-Furanone	52.0	1.2
1,2-Cyclopentanedione	53.5	3.5
1,2-Cyclopentanedione, 3-methyl-	56.7	1.6
Cyclopropyl carbinol	70.1	0.9
1,4-Dioxaspiro[2.4]heptan-5-one, 6-methyl-	72.3	0.8
4-Methyl-2-oxopentanenitrile	75.9	0.8
2,3-Anhydro-d-mannosan	76.2	0.8
Pentanoic acid, 4-oxo-	78.3	0.8
1,4:3,6-Dianhydro-.alpha.-d-glucopyranose	79.9	0.8
5-Hydroxymethylfurfural	82.6	1.8
.beta.-D-Glucopyranose, 1,6-anhydro-	98.2	36.5

Table S5 Specific bio-oil compounds measured by GC-MS with ZSM-5 catalyst

Compound name	Ret. Time (min)	Area percentage %
2-Propen-1-ol	8.1	1.3
3-Penten-2-one, (E)-	8.3	2.1
Cyclopentanone	11.1	0.6
2-Propanone, 1-hydroxy-	21.1	16.4
2-Cyclopenten-1-one	25.6	2.2
1-Hydroxy-2-butanone	27.9	1.5
Acetic acid	33.8	5.6
Furfural	35.6	13.1
Propanoic acid, 2-oxo-, methyl ester	36.2	1.7
2-Propanone, 1-(acetyloxy)-	36.4	1.2
Ethanone, 1-(2-furanyl)-	38.1	1.6
Propanoic acid, ethenyl ester	40.7	0.8
Propanoic acid	40.8	3.8
2-Furancarboxaldehyde, 5-methyl-	42.7	5.1
Butyrolactone	45.2	0.9
Butanoic acid	46.5	2.2
2-Furanmethanol	48.6	3.0
4-Methyl-2-oxo-(1H)-pyrimidine	49.4	0.9
2(5H)-Furanone	52.7	0.7
1,2-Cyclopentanedione	54.1	4.0
2-Butenoic acid, (E)-	54.8	0.6
2-Cyclopenten-1-one, 2-hydroxy-3-methyl-	57.3	2.2
Phenol	67.9	1.0
Phenol, 2-methyl-	68.0	1.1
Cyclopropyl carbinol	70.7	0.7
Phenol, 3-methyl-	71.6	0.5
Pentanoic acid, 4-oxo-	78.7	0.6
1,4:3,6-Dianhydro-.alpha.-d-glucopyranose	80.3	1.0
5-Hydroxymethylfurfural	83.0	3.1
.beta.-D-Glucopyranose, 1,6-anhydro-	98.5	20.5

Table S6 Specific bio-oil compounds measured by GC-MS with Ni_2Fe_3/ZSM-5 catalyst

Compound name	Ret. Time (min)	Area percentage %
3-Penten-2-one, (E)	8.3	2.2
2-Propen-1-ol	8.4	1.1
2-Propanone, 1-hydroxy-	21.4	23.7
2-Cyclopenten-1-one	25.6	2.1
2-Cyclopenten-1-one, 2-methyl-	26.8	1.0
1-Hydroxy-2-butanone	28.0	1.4
Acetic acid	33.6	5.2
Furfural	35.6	12.4
Propanoic acid, 2-oxo-, methyl ester	36.2	1.1
2-Propanone, 1-(acetyloxy)-	36.4	1.5
Ethanone, 1-(2-furanyl)-	38.1	1.3
Formic acid	38.2	1.3
Propanoic acid	40.6	2.3
2-Butanone, 1-(acetyloxy)	40.9	1.4
2-Furancarboxaldehyde, 5-methyl-	42.7	3.9
Propanoic acid, 2-methyl-	42.8	0.6
Butyrolactone	45.2	1.1
Butanoic acid	46.5	2.2
2-Furanmethanol	48.6	2.3
2(5H)-Furanone	52.7	0.8
6-Oxa-bicyclo[3.1.0]hexan-3-one	54.1	4.6
2-Cyclopenten-1-one, 2-hydroxy-3-methyl-	57.2	2.5
Phenol	67.8	0.8
Phenol, 2-methyl-	68.0	0.6
Cyclopropyl carbinol	70.6	0.9
2,3-Anhydro-d-mannosan	76.7	0.6
Decane, 5,6-dimethyl-	79.7	0.4
1,4:3,6-Dianhydro-.alpha.-d-glucopyranose	80.3	1.0
5-Hydroxymethylfurfural	82.9	2.3
.beta.-D-Glucopyranose, 1,6-anhydro-	98.5	17.4