Tuning the activity of $NbOPO_4$ with NiO for selective conversion of cyclohexanone as a model intermediate of lignin pyrolysis bio-oils

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Tables S1-S3 show GC-MS of liquid products from catalytic aldol condensation of cyclohexanone using $NbOPO_4$, 10 wt%NiO/$NbOPO_4$, and 30 wt%NiO/$NbOPO_4$ catalysts at 160°C temperature, 3 h reaction time, 0.5 g loading of catalyst, and 10 bar initial hydrogen pressure.

Table S1. GC-MS of liquid product from catalytic aldol condensation of cyclohexanone using $NbOPO_4$ catalyst at 160°C temperature, 3 h reaction time, 0.5 g loading of catalyst, and 10 bar initial hydrogen pressure.

Compounds	Area	Area%
Cyclohexane	20396187	1.06
Cyclohexene	23868002	1.24
Cyclohexanone	413195810	21.47
Benzene, cyclohexyl-	2246094	0.12
1-Adamantyl methyl ketone	3175733	0.17
Bicyclopentyl-1,1'-diene	3158617	0.16
[1,1'-Bicyclohexyl]-2-one	19944919	1.04
1(2H)-Naphthalenone, 3,4-dihydro-6-methoxy-	19428291	1.01
Tricyclo[5.3.1.1(2,6)]dodecan-11-one	59604528	3.1
Cyclohexanone, 2-cyclohexylidene-	688604699	35.79
Cyclohexanone, 2-(1-cyclohexen-l-yl)-	130166217	6.76
Pentylidenecyclohexane	2796610	0.15
Cyclohexene, 3-pentyl-	34309294	1.78
[1,1'-Bicyclohexyl]-2-one	4955545	0.26
Benzene, (2-cyclohexyl-1-cyclohexen-1-yl)-	4999461	0.26
2,6-Naphthalenediol, bis(4-pentylbenzoate)	311852512	16.21
Cyclohexanone, 2-cyclohexylidene-	67911651	3.53
Triphenylene, 1,2,3,4,5,6,7,8,9,10,11,12-dodecahydro-	108380199	5.63
9,12,15-Octadecatrienoic acid, ethyl ester, (Z,Z,Z)-	1613024	0.08
7-Octylidenebicyclo[4.1.0]heptane	3562682	0.19

Table S2. GC-MS of liquid product from catalytic aldol condensation of cyclohexanone using 10 wt%NiO/$NbOPO_4$ catalyst at 160°C temperature, 3 h reaction time, 0.5 g loading of catalyst, and 10 bar initial hydrogen pressure.

Compounds	**Area**	**Area%**
1-Butanol	5818495	0.31
Cyclohexene	429054	0.02
Cyclohexanone	832585959	45
Benzene, (1-methylethyl)-	223080	0.01
Cyclohexanone, 2-(2-methylpropylidene)-	249998	0.01
1-Adamantyl methyl ketone	731834	0.04
[1,1'-Bicyclohexyl]-2-one	942525	0.05
1(2H)-Naphthalenone, 3,4-dihydro-6-methoxy-	1619764	0.09
Cyclohexanone, 2-cyclohexylidene-	789146451	42.65
Cyclohexanone, 2-(1-cyclohexen-l-yl)-	179959390	9.73
2-Sec-Butylcyclohexanone	5997631	0.32
Tricyclo[6.3.0.0(1,5)]undecan-4-one, 5,9-dimethyl-	385904	0.02
Benzene, (2-cyclohexyl-1-cyclohexen-1-yl)-	209689	0.01
Benzoic acid, 4-(4-ethylcyclohexyl)-, 2,3-dicyano-4-ethoxyphenyl ester	232677	0.01
Benzene, (2-cyclohexyl-1-cyclohexen-1-yl)-	236947	0.01
1,4-Methanobenzocyclodecene, 1,2,3,4,4a,5,8,9,12,12a-decahydro-	2652551	0.14
1,4-Methanobenzocyclodecene, 1,2,3,4,4a,5,8,9,12,12a-decahydro-	23905041	1.29
2,6-Naphthalenediol, bis(4-pentylbenzoate)	929211	0.05
Triphenylene, 1,2,3,4,5,6,7,8,9,10,11,12-dodecahydro-	4069954	0.22

Table S3. GC-MS of liquid product from catalytic aldol condensation of cyclohexanone using 30 wt%NiO/$NbOPO_4$ catalyst at 160°C temperature, 3 h reaction time, 0.5 g loading of catalyst, and 10 bar initial hydrogen pressure.

Compounds	Area	Area%
1-Butanol	245006	0.01
Cyclohexane	607754	0.03
Cyclohexene	765072	0.04
Heptane, 2,5-dimethyl-	256374	0.01
Cyclohexanol	308372	0.02
Cyclohexanol	619321130	35.61
Cyclohexanone	307080594	17.66
Benzene, (1-methylethyl)-	217197	0.01
Cyclohexanone, 2-butyl-	343053	0.02
1-Bromoadamantane	388776	0.02
[1,1'-Bicyclohexyl]-2-one	23587640	1.36
1(2H)-Naphthalenone, 3,4-dihydro-6-methoxy-	2113010	0.12
Cyclohexanone, 2-cyclohexylidene-	622520455	35.79
Cyclohexanone, 2-(1-cyclohexen-l-yl)-	137032529	7.88
7-Tetradecenal, (Z)-	187256	0.01
2-Sec-Butylcyclohexanone	6261827	0.36
Tricyclo[6.3.0.0(1,5)]undecan-4-one, 5,9-dimethyl-	640195	0.04

1,4-Methanobenzocyclodecene, 1,2,3,4,4a,5,8,9,12,12a-decahydro-	1724534	0.1
1,4-Methanobenzocyclodecene, 1,2,3,4,4a,5,8,9,12,12a-decahydro-	13161032	0.76
2,6-Naphthalenediol, bis(4-pentylbenzoate)	690338	0.04
Triphenylene, 1,2,3,4,5,6,7,8,9,10,11,12-dodecahydro-	1810112	0.1