

Supporting Information

Light Cycle Oil Upgrading to Benzene, Toluene and Xylenes by Hydrocracking: Studies Using Model Mixtures

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Table S1. Hydrogenation of naphthalene under various reaction conditions and over different catalysts.

Catalyst	Solvent	Temperature (°C)	Pressure (MPa)	Products	Ref.
NiW/Al ₂ O ₃	Crude	350-370	4	At 2 MPa: naphthalene (25-11%), tetralin (75-89%) At 4 MPa: naphthalene (10-5%), tetralin (90-95%)	13
ATTM*	None	350-450	6.3-7.1	At 160 min, 350-450 °C: naphthalene (47-27%), tetralin (53-73%)	14
Ni/Al ₂ O ₃	Decane	80-160	2-4	At 2 MPa, 130 °C: naphthalene (24 %), tetralin (67%), decalins (8%), octalin (1%)	15
M=Rh, Pt, Ir, Ru on SiAl ₂ O (2MSiAl ₂ O)	None	200-300	Atm.	At 200 °C: Rh: naphthalene (3.7%), tetralin (94.1%), decalin (2.2%). Pt: naphthalene (0%), tetralin (2.6%), decalin (97.4%). Ir: naphthalene (4.2%), tetralin (80.0%), decalin (15.6%), others (0.2%). Ru: naphthalene (5.0%), tetralin (92.3%), decalin (2.5%), others (0.2%)	16
Fe ₂ (MoO ₄) ₃	Formic acid	274-333		At 333 °C, 0.28 mL formic acid, 5 h: tetralin (85%), decalin (7.5%), coke (7.5%), water density 0.082 g mL ⁻¹	17
MoP/support		300	4	MoP/HZSM5: conversion 60%, tetralin 27% MoP/Hbeta: conversion 90%, tetralin 58% MoP/HY: conversion 85%, tetralin 99%	18
Mo ₂ C-support	<i>n</i> -heptane	250-400	3-4	Mo ₂ C(20)/Al ₂ O ₃ : naphthalene (1%), tetralin (99%) Mo ₂ C(10)/Al ₂ O ₃ : naphthalene (7.6 %), tetralin Mo ₂ C(5)/Al ₂ O ₃ : naphthalene (9 %), tetralin (90.5%), decalin (0.5%)	8

* Ammonium tetrathiomolybdate

Table S2. Hydrogenation of naphthalene derivatives under various reaction conditions and over different catalysts.

Model	Catalyst	Solvent	Temperature (°C)	Pressure (MPa)	Products	Ref.
1-methylnaphthalene	NiW/USY	Cyclohexane	350	19.3 (6.9)	At 300 min: 1-methylnaphthalene (5%), 2-methylnaphthalene (5%), methyltetralins (86%), methyldecalins, penthyl benzene (4%)	24
1-methylnaphthalene	CoMo/Al ₂ O ₃	Tetradecane, pentadecane, hexadecane	310-370	5-8 (3.1-7.5 H ₂)	At 330 °C, 3.1-7.5 MPa: methyltetralin (88-60%), methyldecalin (12-40%) At 6.5 MP At 310-350 °C: methyltetralin (87-33%), methyldecalin (13-66%).	26
2-methylnaphthalene	Mo ₂ C-support	<i>n</i> -heptane	250-400	3-4	Mo ₂ C(20)/g-Al ₂ O ₃ : At 250 °C: 2-methylnaphthalene (2.8%), 2-methyltetralin (24.8%), 6-methyltetralin (72.4%). At 300 °C: 2-methylnaphthalene (10.6%), 2-methyltetralin (25.8%), 6-methyltetralin (63.6%).	8
1-methylnaphthalene, dimethyl disulfide, methylamine	NiMoP/Al ₂ O ₃	<i>n</i> -heptane	400	2.8	1-methylnaphthalene (37.9 %), 2-methylnaphthalene (6.3 %), methyltetralins (42.1 %), methyldecalins (5.2 %), alkylindanes (2 %), alkylbenzenes (3.2 %), naphthalene (1.2 %), tetralin (1.7).	27

Table S3 Hydrocracking of naphthalene and naphthalene derivatives under various reaction conditions and over different catalysts.

Model	Catalyst	Solvent	Temperature (°C)	Pressure (MPa)	Products	Ref.
Naphthalene	USY	None	400-600	5	At 600 °C: C ₁ -C ₇ gases (70%), benzene (25%), toluene (9%), xylene (1%)	28
1-Methylnaphthalene	USY	None	400-600	5	At 600 °C: C ₁ -C ₃ gases (60%), benzene (35%), toluene (10%), xylene (1%)	28
Naphthalene	Ni ₂ P/HZSM5, Ni ₂ P/Beta, Ni ₂ P/USY	Tridecane	400	3	Ni ₂ P/Beta: naphthalene (1%), BTX (94.4%), others (4.6%).	29
Naphthalene	Mixture of FeSO ₄ H ₂ O (20 wt.%), Fe ₂ O ₃ (20 wt.%), Al ₂ O ₃ (20 wt.%) and sulfur (40 wt.%)	Solvent mixture	400-450	5, 10, 12	At 10 MPa, 450 °C, 90 min: benzene (37%), toluene (34%), ethylbenzene (10%), indan (1%), 1-methylindan (0.5%), tetralin (1.5%), naphthalene (16%). At 12 MPa, 450 °C, 90 min: benzene (28%), toluene (17%), ethylbenzene (16%), indan (4%), butylbenzene (0.2%), 1-methylindan (4%), tetralin (2%), naphthalene (28.5%).	30
1-Methylnaphthalene	Ni ₂ P/Beta nano Ni ₂ P/Beta micro		380	6	Ni ₂ P/Beta nano: 1-methyl naphthalene (1%), BTX (42.3%), others (57.7%) Ni ₂ P/Beta micro: 1-methyl naphthalene (1%), BTX (30.5%), others (65.5%).	31

Table S4. Hydrocracking of tetralin under various reaction conditions and over different catalysts.

Catalyst	Solvent	Temperature (°C)	Pressure (MPa)	WHSV (h ⁻¹)	Products	Ref.
HY		400	0.0		More than 20 products	32,33
HZSM5 (Si/Al=105)		400	0.0		C ₃ gas, benzene, toluene, ethylbenzene, xylenes, naphthalene	33
USY		400-600	5		C ₁ -C ₃ gases (64 %), benzene (30 %), toluene (7 %)	33
NiW/USY, NiW/HY, NiW/mordenite		400	6.1		Gas, benzene monoaromatics, decalin, decalin isomers, metil indan, indan, naphthalene	35
USY, NiW/USY, NiW/Al ₂ O ₃		250-300	6.1		Gas, benzene, alkyl benzene, mono cyclo paraffins, decalin, indan, methyl indan	36
H-Beta, Ni/H-Beta	<i>n</i> -heptane	450	4.0	2	Benzene, toluene, xylene	8
Ni-H (Sn)/Beta	<i>n</i> -heptane	425-450	4.0	2	Benzene, toluene, xylene	37
CoMo/Beta	<i>n</i> -heptane	370	8.0	1.6	C1-C4 (21.6%), Benzene (25%), toluene (16.5%), xylene (12.7), C9 (5.3%), C10 (3.1%)	38