Assessing supported nickel catalysts for the upcycling of real

WEEE plastics through low-pressure hydropyrolysis and

dehalogenation

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Supplementary Information



Figure S1. N₂ adsorption-desorption Isotherms (77 K): (A) Ni/n-ZSM-5 and Ni/AC (points), and supports (lines); (B) Ni/Al₂O₃ and Ni/SiO₂ (points) and supports (lines); (C) Pore Size Distributions calculated by BJH model for Ni/Al₂O₃ and Ni/SiO₂.



Figure S2. Powder XRD patterns of Ni-based catalysts (colored) and supports (grey): (A) Ni/Al₂O₃, (B) Ni/n-ZSM-5, (C) Ni/SiO₂ and (D) Ni/AC.



Figure S3. NH₃-TPD profiles of Ni/Al₂O₃ and Ni/n-ZSM-5 catalysts.



Figure S4. Hourly results obtained in the hydrotreatment (350 °C and 6 bar) of the WEEE plastics pyrolysis oil (Feed 2) over Ni/AC fresh and regenerated catalysts using a continuous reaction system: (A) Yield of oil components grouped by families and (B) Yield of GC-MS detected and non-detected oil fractions. Grey bars correspond with the raw pyrolysis oil.



Figure S5. Particle size distributions for fresh and regenerated Ni/AC.



Figure S6. TG-Ar analysis of fresh, spent and regenerated Ni/AC catalysts.

Table S1. Main compounds detected in the oils produced in the hydropyrolysis experiments.

Compound	Family
Ethylbenzene	M-AR
Styrene	M-AR
.alphaMethylstyrene	M-AR
Toluene	M-AR
Benzene, (1-methylethyl)-	M-AR
Benzene, (1,3-dimethyl-3-butenyl)-	M-AR
Benzene, propyl-	M-AR
Benzene, cyclopropyl-	M-AR
Benzene	M-AR
Benzene, heptyl-	M-AR
Benzene, n-butyl-	M-AR
Benzene, (2,3-dimethyldecyl)-	M-AR
Xylene	M-AR
Benzene, 1-methyl-4-propyl-	M-AR
Benzene, 1,2,4-trimethyl-	M-AR
Indane	M-AR
Mesitylene	M-AR
1H-Indene, 2,3-dihydro-4-methyl-	M-AR
2-Methylindene	M-AR
Benzene, 1-ethenyl-3,5-dimethyl-	M-AR
Benzene, 1,2,3,5-tetramethyl-	M-AR
Benzene, 1-ethyl-2-methyl-	M-AR
Cycloprop[a]indene, 1,1a,6,6a-tetrahydro-	M-AR
Benzene, 1,1'-(1,3-propanediyl)bis-	P-AR
1-Isopropenylnaphthalene	P-AR
Acenaphthene	P-AR
1,1'-Biphenyl, 4-methyl-	P-AR
Naphthalene	P-AR
Bibenzyl	P-AR
Naphthalene, 2-methyl-	P-AR
Benzene, 1,1'-(1-methyl-1,3-propanediyl)bis-	P-AR
Naphthalene, 1,3-dimethyl-	P-AR
1,1'-Biphenyl, 3-methyl-	P-AR
Benzene, 1,1'-ethylidenebis-	P-AR
Naphthalene, 1-phenyl-	P-AR
1,2-Diphenylcyclopropane	P-AR
Acephenanthrylene, 4,5-dihydro-	P-AR
Naphthalene, 1,2,3,4-tetrahydro-	P-AR
Naphthalene, 1,2,3,4-tetrahydro-2-phenyl-	P-AR
Naphthalene, 1,2-dihydro-	P-AR

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Cyclopentane, 1-butyl-2-propyl-ALIPHCyclohexaneALIPHPentane, 2-methyl-ALIPH1-Butene, 2,3-dimethyl-ALIPH1-Butene, 2,3-dimethyl-ALIPHNonane, 2,6-dimethyl-ALIPHHeptane, 4-methyl-ALIPH2-Pentene, 3,4-dimethyl-, (E)-ALIPHPentadecaneALIPHDodecaneALIPHTridecaneALIPHCyclopentylcyclohexaneALIPHCyclopentylcyclohexaneALIPH1-Ethyl-3-methylcyclohexane (c,t)ALIPHDodecane, 1-cyclopentyl-4-(3-cyclopentylpropyl)-ALIPHCyclopentane, 1,1'-[3-(2-cyclopentylpropyl)-ALIPHCyclopentane, 1,1'-[3-(2-cyclopentylpropyl)-ALIPH1-Ethyl-4-methylcyclohexaneALIPH1-Ethyl-4-methylcyclohexaneALIPH1-Ethyl-4-methylcyclohexaneALIPH1-Undecene, 7-methyl-ALIPH1-Undecene, 7-methyl-ALIPH1,3-Pentadiene, 2,4-dimethyl-ALIPH1,12-TridecadieneALIPH1,12-TridecadieneALIPH1,12-TridecadieneALIPH	Pentane	ALIPH
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Pentane, 2-methyl-ALIPH1-Butene, 2,3-dimethyl-ALIPH1-Butene, 2,3-dimethyl-ALIPHNonane, 2,6-dimethyl-ALIPHHeptane, 4-methyl-ALIPH2-Pentene, 3,4-dimethyl-, (E)-ALIPHPentadecaneALIPHDodecaneALIPHTridecaneALIPHCyclopentylcyclohexaneALIPHCyclopentylcyclohexane (c,t)ALIPH1-Ethyl-3-methylcyclohexane (c,t)ALIPHDodecane, 1-cyclopentyl-4-(3-cyclopentylpropyl)-ALIPHCyclopentane, 1,1'-[3-(2-cyclopentylethyl)-1,5-pentanediyl]bis-ALIPH1-Ethyl-4-methylcyclohexaneALIPH1-Ethyl-4-methylcyclohexaneALIPH1-Ethyl-4-methylcyclohexaneALIPH1-Ethyl-4-methylcyclohexaneALIPH1-Ethyl-4-methylcyclohexaneALIPH1-Ethyl-4-methylcyclohexaneALIPH1-Ethyl-4-methylcyclohexaneALIPH1-Ethyl-4-methylcyclohexaneALIPH1-Ethyl-4-methylcyclohexaneALIPH1-Ethyl-4-methylcyclohexaneALIPH1-Undecene, 7-methyl-ALIPH1-Undecene, 7-methyl-ALIPH1,3-Pentadiene, 2,4-dimethyl-ALIPH1,12-TridecadieneALIPH1,12-TridecadieneALIPHCyclohexaneALIPH1,12-TridecadieneALIPH1,12-TridecadieneALIPH1,12-TridecadieneALIPH1,12-TridecadieneALIPH1,12-TridecadieneALIPH	Cyclohexane	ALIPH
1-Butene, 2,3-dimethyl-ALIPHNonane, 2,6-dimethyl-ALIPHHeptane, 4-methyl-ALIPH2-Pentene, 3,4-dimethyl-, (E)-ALIPHPentadecaneALIPHDodecaneALIPHTridecaneALIPHCyclopentylcyclohexaneALIPHCyclopentylcyclohexaneALIPH1-Ethyl-3-methylcyclohexane (c,t)ALIPHDodecane, 1-cyclopentyl-4-(3-cyclopentylpropyl)-ALIPHDodecane, 1-cyclopentyl-4-(3-cyclopentylpropyl)-ALIPHCyclopentane, 1,1'-[3-(2-cyclopentylethyl)-1,5-pentanediyl]bis-ALIPH1-Ethyl-4-methylcyclohexaneALIPH1-Ethyl-4-methylcyclohexaneALIPH1-Undecene, 7-methyl-ALIPH1-Undecene, 7-methyl-ALIPH1,3-Pentadiene, 2,4-dimethyl-ALIPH1,12-TridecadieneALIPHCyclopentane, 14 dimethylALIPHCyclopentane, 14 dimethylALIPH	Pentane, 2-methyl-	ALIPH
Nonane, 2,6-dimethyl-ALIPHHeptane, 4-methyl-ALIPH2-Pentene, 3,4-dimethyl-, (E)-ALIPHPentadecaneALIPHDodecaneALIPHTridecaneALIPHCyclopentylcyclohexaneALIPHCyclohexane, (1-methylethyl)-ALIPH1-Ethyl-3-methylcyclohexane (c,t)ALIPHDodecane, 1-cyclopentyl-4-(3-cyclopentylpropyl)-ALIPHCyclopentane, 1,1'-[3-(2-cyclopentylpropyl)-ALIPHCyclopentane, 1,1'-[3-(2-cyclopentylpropyl)-ALIPH1-Ethyl-4-methylcyclohexaneALIPH1-Ethyl-4-methylcyclohexaneALIPH1-Ethyl-4-methylcyclohexaneALIPH1-Undecene, 7-methyl-ALIPH1-Undecene, 7-methyl-ALIPH1,3-Pentadiene, 2,4-dimethyl-ALIPH1,12-TridecadieneALIPHCyclohexane, 14 dimethylALIPH	1-Butene, 2,3-dimethyl-	ALIPH
Heptane, 4-methyl-ALIPH2-Pentene, 3,4-dimethyl-, (E)-ALIPHPentadecaneALIPHPentadecaneALIPHDodecaneALIPHTridecaneALIPHCyclopentylcyclohexaneALIPHCyclohexane, (1-methylethyl)-ALIPH1-Ethyl-3-methylcyclohexane (c,t)ALIPHDodecane, 1-cyclopentyl-4-(3-cyclopentylpropyl)-ALIPHCyclopentane, 1,1'-[3-(2-cyclopentylpropyl)-ALIPH7-Octadecyne, 2-methyl-ALIPH1-Ethyl-4-methylcyclohexaneALIPH1-Ethyl-4-methylcyclohexaneALIPH1-Undecene, 7-methyl-ALIPH1-Undecene, 7-methyl-ALIPH1,3-Pentadiene, 2,4-dimethyl-ALIPH1,12-TridecadieneALIPH1,12-TridecadieneALIPH1,12-TridecadieneALIPH	Nonane, 2,6-dimethyl-	ALIPH
2-Pentene, 3,4-dimethyl-, (E)-ALIPHPentadecaneALIPHPentadecaneALIPHDodecaneALIPHTridecaneALIPHCyclopentylcyclohexaneALIPHCyclohexane, (1-methylethyl)-ALIPH1-Ethyl-3-methylcyclohexane (c,t)ALIPHDodecane, 1-cyclopentyl-4-(3-cyclopentylpropyl)-ALIPHCyclopentane, 1,1'-[3-(2-cyclopentylpropyl)-ALIPHCyclopentane, 1,1'-[3-(2-cyclopentylethyl)-1,5-pentanediyl]bis-ALIPH7-Octadecyne, 2-methyl-ALIPH1-Ethyl-4-methylcyclohexaneALIPH1-Ethyl-4-methylcyclohexaneALIPH1-Undecene, 7-methyl-ALIPH1-Undecene, 7-methyl-ALIPH1,3-Pentadiene, 2,4-dimethyl-ALIPH1,12-TridecadieneALIPH1,12-TridecadieneALIPH	Heptane, 4-methyl-	ALIPH
PentadecaneALIPHDodecaneALIPHDodecaneALIPHTridecaneALIPHCyclopentylcyclohexaneALIPHCyclohexane, (1-methylethyl)-ALIPH1-Ethyl-3-methylcyclohexane (c,t)ALIPHDodecane, 1-cyclopentyl-4-(3-cyclopentylpropyl)-ALIPHCyclopentane, 1,1'-[3-(2-cyclopentylpropyl)-ALIPH7-Octadecyne, 2-methyl-ALIPH1-Ethyl-4-methylcyclohexaneALIPH1-Ethyl-4-methylcyclohexaneALIPH1-Undecene, 7-methyl-ALIPH1-Undecene, 7-methyl-ALIPH1,3-Pentadiene, 2,4-dimethyl-ALIPH1,12-TridecadieneALIPH1,12-TridecadieneALIPH	2-Pentene, 3,4-dimethyl-, (E)-	ALIPH
DodecaneALIPHTridecaneALIPHTridecaneALIPHCyclopentylcyclohexaneALIPHCyclohexane, (1-methylethyl)-ALIPH1-Ethyl-3-methylcyclohexane (c,t)ALIPHDodecane, 1-cyclopentyl-4-(3-cyclopentylpropyl)-ALIPHCyclopentane, 1,1'-[3-(2-cyclopentylethyl)-1,5-pentanediyl]bis-ALIPH7-Octadecyne, 2-methyl-ALIPH1-Ethyl-4-methylcyclohexaneALIPH1-Ethyl-4-methylcyclohexaneALIPH1-Undecene, 7-methyl-ALIPH1-Undecene, 7-methyl-ALIPH1,3-Pentadiene, 2,4-dimethyl-ALIPH1,12-TridecadieneALIPH1,12-TridecadieneALIPH	Pentadecane	ALIPH
TridecaneALIPHCyclopentylcyclohexaneALIPHCyclohexane, (1-methylethyl)-ALIPH1-Ethyl-3-methylcyclohexane (c,t)ALIPHDodecane, 1-cyclopentyl-4-(3-cyclopentylpropyl)-ALIPHCyclopentane, 1,1'-[3-(2-cyclopentylethyl)-1,5-pentanediyl]bis-ALIPH7-Octadecyne, 2-methyl-ALIPH1-Ethyl-4-methylcyclohexaneALIPHm-Menthane, (15,35)-(+)-ALIPH1-Undecene, 7-methyl-ALIPH1-Undecene, 7-methyl-ALIPH1,3-Pentadiene, 2,4-dimethyl-ALIPH1,12-TridecadieneALIPH1,12-TridecadieneALIPH	Dodecane	ALIPH
CyclopentylcyclohexaneALIPHCyclohexane, (1-methylethyl)-ALIPH1-Ethyl-3-methylcyclohexane (c,t)ALIPHDodecane, 1-cyclopentyl-4-(3-cyclopentylpropyl)-ALIPHCyclopentane, 1,1'-[3-(2-cyclopentylethyl)-1,5-pentanediyl]bis-ALIPH7-Octadecyne, 2-methyl-ALIPH1-Ethyl-4-methylcyclohexaneALIPH1-Ethyl-4-methylcyclohexaneALIPH1-Undecene, 7-methyl-ALIPH1-Undecene, 7-methyl-ALIPH1,3-Pentadiene, 2,4-dimethyl-ALIPH1,12-TridecadieneALIPH1,12-TridecadieneALIPH	Tridecane	ALIPH
Cyclohexane, (1-methylethyl)-ALIPH1-Ethyl-3-methylcyclohexane (c,t)ALIPHDodecane, 1-cyclopentyl-4-(3-cyclopentylpropyl)-ALIPHCyclopentane, 1,1'-[3-(2-cyclopentylethyl)-1,5-pentanediyl]bis-ALIPH7-Octadecyne, 2-methyl-ALIPH1-Ethyl-4-methylcyclohexaneALIPHm-Menthane, (1S,3S)-(+)-ALIPH1-Undecene, 7-methyl-ALIPH1-Undecene, 7-methyl-ALIPH1,3-Pentadiene, 2,4-dimethyl-ALIPH1,12-TridecadieneALIPH	Cyclopentylcyclohexane	ALIPH
1-Ethyl-3-methylcyclohexane (c,t)ALIPHDodecane, 1-cyclopentyl-4-(3-cyclopentylpropyl)-ALIPHCyclopentane, 1,1'-[3-(2-cyclopentylethyl)-1,5-pentanediyl]bis-ALIPH7-Octadecyne, 2-methyl-ALIPH1-Ethyl-4-methylcyclohexaneALIPH1-Ethyl-4-methylcyclohexaneALIPHm-Menthane, (15,35)-(+)-ALIPH1-Undecene, 7-methyl-ALIPH1-Undecene, 7-methyl-ALIPH1,3-Pentadiene, 2,4-dimethyl-ALIPH1,12-TridecadieneALIPH1,12-TridecadieneALIPH	Cyclohexane, (1-methylethyl)-	ALIPH
Dodecane, 1-cyclopentyl-4-(3-cyclopentylpropyl)-ALIPHCyclopentane, 1,1'-[3-(2-cyclopentylethyl)-1,5-pentanediyl]bis-ALIPH7-Octadecyne, 2-methyl-ALIPH1-Ethyl-4-methylcyclohexaneALIPHm-Menthane, (15,35)-(+)-ALIPH1-Undecene, 7-methyl-ALIPHTetracyclo[5.3.0.0<2,6>.0<3,10>]deca-4,8-dieneALIPH1,3-Pentadiene, 2,4-dimethyl-ALIPH1,12-TridecadieneALIPH1,12-TridecadieneALIPH	1-Ethyl-3-methylcyclohexane (c,t)	ALIPH
Cyclopentane, 1,1'-[3-(2-cyclopentylethyl)-1,5-pentanediyl]bis-ALIPH7-Octadecyne, 2-methyl-ALIPH1-Ethyl-4-methylcyclohexaneALIPHm-Menthane, (15,3S)-(+)-ALIPH1-Undecene, 7-methyl-ALIPHTetracyclo[5.3.0.0<2,6>.0<3,10>]deca-4,8-dieneALIPH1,3-Pentadiene, 2,4-dimethyl-ALIPH1,12-TridecadieneALIPHCyclohexane1.4 dimethyl	Dodecane, 1-cyclopentyl-4-(3-cyclopentylpropyl)-	ALIPH
7-Octadecyne, 2-methyl-ALIPH1-Ethyl-4-methylcyclohexaneALIPH1-Ethyl-4-methylcyclohexaneALIPHm-Menthane, (1S,3S)-(+)-ALIPH1-Undecene, 7-methyl-ALIPH1-Undecene, 7-methyl-ALIPHTetracyclo[5.3.0.0<2,6>.0<3,10>]deca-4,8-dieneALIPH1,3-Pentadiene, 2,4-dimethyl-ALIPH1,12-TridecadieneALIPHCyclohovano, 1.4 dimethylALIPH	Cyclopentane, 1,1'-[3-(2-cyclopentylethyl)-1,5-pentanediyl]bis-	ALIPH
1-Ethyl-4-methylcyclohexaneALIPHm-Menthane, (15,35)-(+)-ALIPH1-Undecene, 7-methyl-ALIPHTetracyclo[5.3.0.0<2,6>.0<3,10>]deca-4,8-dieneALIPH1,3-Pentadiene, 2,4-dimethyl-ALIPH1,12-TridecadieneALIPHCyclohovana, 1.4 dimethylALIPH	7-Octadecyne, 2-methyl-	ALIPH
m-Menthane, (15,3S)-(+)-ALIPH1-Undecene, 7-methyl-ALIPHTetracyclo[5.3.0.0<2,6>.0<3,10>]deca-4,8-dieneALIPH1,3-Pentadiene, 2,4-dimethyl-ALIPH1,12-TridecadieneALIPHCycloboxano, 1.4 dimethylALIPH	1-Ethyl-4-methylcyclohexane	ALIPH
1-Undecene, 7-methyl-ALIPHTetracyclo[5.3.0.0<2,6>.0<3,10>]deca-4,8-dieneALIPH1,3-Pentadiene, 2,4-dimethyl-ALIPH1,12-TridecadieneALIPHCycloboxane, 1.4 dimethylALIPH	m-Menthane, (1S,3S)-(+)-	ALIPH
Tetracyclo[5.3.0.0<2,6>.0<3,10>]deca-4,8-dieneALIPH1,3-Pentadiene, 2,4-dimethyl-ALIPH1,12-TridecadieneALIPHCycloboxano, 1.4 dimethylALIPH	1-Undecene, 7-methyl-	ALIPH
1,3-Pentadiene, 2,4-dimethyl-ALIPH1,12-TridecadieneALIPHCycloboxane, 1.4 dimethylALIPH	Tetracyclo[5.3.0.0<2,6>.0<3,10>]deca-4,8-diene	ALIPH
1,12-Tridecadiene ALIP	1,3-Pentadiene, 2,4-dimethyl-	ALIPH
Cudobovana 1.4 dimethul	1,12-Tridecadiene	ALIPH
Cyclonexane, 1,4-annechyi- ALIPh	Cyclohexane, 1,4-dimethyl-	ALIPH

Compound	Family
Phenol, 3-(1-methylethyl)-	O-Comp
Phenol	O-Comp
Naphthalene-1,4-diol, 4-O-benzoyl(ether)	O-Comp
1-Octanol, 2-butyl-	O-Comp
Phenol, 2-methyl-	O-Comp
Phenol, 3,5-dimethyl-	O-Comp
Methyl methacrylate	O-Comp
Phenol, 2,4-dimethyl-	O-Comp
11,13-Dimethyl-12-tetradecen-1-ol acetate	O-Comp
2-Cyclohexen-1-one, 4-ethyl-3,4-dimethyl-	O-Comp
2-Cyclohexene-1-carboxaldehyde, 2,6,6-trimethyl-	O-Comp
2-Isopropyl-5-methyl-1-heptanol	O-Comp
p-Isopropenylphenol	O-Comp
Methyl isobutyrate	O-Comp
p-Cumenol	O-Comp
Benzofuran, 2,3-dihydro-2-methyl-	O-Comp
Phenol, 2,4,6-trimethyl-	O-Comp
11-Methyldodecanol	O-Comp
3,4-Dimethyl cyclohexanone	O-Comp
Phytol	O-Comp
Bicyclo[4.1.0]heptan-2-ol, 1-phenyl-, endo-	O-Comp
Oxirane, trimethyl-	O-Comp
Isopropyl Alcohol	O-Comp
2-Propanone, 1-methoxy-	O-Comp
Benzenebutanenitrile	N-Comp
Methylacrylonitrile	N-Comp
Benzeneacetonitrile, .alphamethyl-	N-Comp
Benzenepropanenitrile	N-Comp
Benzyl nitrile	N-Comp
Propanenitrile	N-Comp
Isobutyronitrile	N-Comp
3-Phenyl-2-pentenenitrile	N-Comp
2-Naphthalenecarbonitrile	N-Comp
Caprolactam	N-Comp
Acridine, 9-phenyl-	N-Comp

Table S2. Main compounds detected in dioxane used for regeneration of Ni/AC spent catalyst.

Compound	Family
Benzene	M-AR
Benzene, 1,2,4-trimethyl-	M-AR
Benzene, 1,3-dimethyl-	M-AR
Benzene, 1,4-diethyl-	M-AR
Benzene, 1-ethyl-2-methyl-	M-AR
Benzene, 1-ethyl-4-methyl-	M-AR
Benzene, 1-methyl-3-(1-methylethyl)-	M-AR
Ethylbenzene	M-AR
Toluene	M-AR
Naphthalene	P-AR
Naphthalene, 2-(1-methylethyl)-	P-AR
Naphthalene, 2,6-dimethyl-	P-AR
Naphthalene, 2-ethyl-	P-AR
Naphthalene, 2-methyl-	P-AR