

Supplementary information

Conversion of low-density polyethylene plastic waste into valuable fuels using fly ash as catalyst

1. Characterization of fly ash

Surface area and pore structures of sample were analyzed by N₂ adsorption/desorption isotherms at 77.3K using a physisorption analyze (quant chrome nova instruments). Moisture and impurities were removed by degassing the ash sample at 120°C for 8 hrs. The Brunauer-Emmett-Teller (BET) theory was used to calculate the specific surface areas. The t-plot method was used to determine the micro pore volume, micro pore, and external surface area. An IR Prestige 21 spectrometer in attenuated total reflection (ATR) mode (Bruker alpha) was used to obtain the FTIR spectra of fly ash sample the spectra were recorded at a range of 500–4000 cm⁻¹ at a resolution of 8cm⁻¹ using a combined 64 scans. The Bruker alpha model was used to determine functional group of fly ash. The scanning electron microscope (SEM) (VEGA3 TESCON) was used to identify the surface morphology of the catalyst. Material. Composition of fly ash was determined by EDS technique with SEM.

Table S1. GCMS result of oil sample with 5% fly ash (P- 500-FA-5)

Retention time	Compound name	formulae	Area%
2.627	Heptane	C ₇ H ₁₆	0.48
2.849	Cyclohexene,4-methyl	C ₇ H ₁₂	0.21
2.912	Cyclohexane, methyl	C ₇ H ₁₄	0.21
3.069	Cyclohexene, 4- methyl	C ₇ H ₁₂	0.32
3.226	Cyclopentene, 3-ethyl-	C ₇ H ₁₂	0.21
3.377	Toluene	C ₇ H ₈	0.89
3.419	Cyclohexene, 1-methy	C ₇ H ₁₄	0.32
3.542	Ethylidenecyclobutane	C ₈ H ₁₂	0.16
3.654	1-Octene	C ₈ H ₁₆	1.51
3.771	Octane	C ₈ H ₁₈	0.64

4.694	Ethylbenzene	C_8H_{10}	0.27
4.828	p-Xylene	C_8H_{10}	0.48
4.991	1,5-Hexadiene	C_6H_{10}	0.24
5.134	1-Nonene	C_9H_{18}	1.74
5.186	o-Xylene	C_8H_{10}	0.29
5.269	Nonane	C_9H_{20}	0.65
6.612	1,9-Decadiene	$C_{10}H_{18}$	0.20
6.751	1-Decene	$C_{10}H_{20}$	2.22
6.891	Decane	$C_{10}H_{22}$	0.64
8.227	Cycloundecene	$C_{11}H_{20}$	0.30
8.360	1-Undecene	$C_{11}H_{22}$	2.14
8.493	Undecane	$C_{11}H_{24}$	0.80
9.775	1,11-Dodecadiene	$C_{12}H_{22}$	0.32
9.898	1-Dodecene	$C_{12}H_{24}$	1.85
10.022	Dodecane	$C_{12}H_{26}$	0.79
11.239	1,13-Tetradecadiene	$C_{13}H_{24}$	0.40
11.352	1-Tridecene	$C_{13}H_{26}$	1.73
11.467	Tridecane	$C_{13}H_{28}$	0.78
12.620	1-Tridecadien	$C_{13}H_{24}$	0.39
12.725	2-Tetradecene,	$C_{14}H_{28}$	1.84
12.829	Tetradecane	$C_{14}H_{30}$	0.76
13.925	1,13-Tetradecadiene	$C_{14}H_{26}$	0.33
14.020	Pentadecene	$C_{15}H_{30}$	1.65

14.115	Pentadecane	$C_{15}H_{32}$	0.75
15.158	1,13-Tetradecadiene	$C_{14}H_{24}$	0.32
15.245	1-Octadecanol	$C_{18}H_{38}$	1.47
15.331	Hexadecane	$C_{16}H_{34}$	0.79
16.326	Nonadecen-1-ol	$C_{19}H_{40}$	0.29
16.407	Heptadecene	$C_{17}H_{34}$	1.31
16.486	Heptadecane	$C_{17}H_{36}$	0.66
17.438	1,15-Hexadecadiene	$C_{16}H_{30}$	0.27
17.511	1-Heptadecene	$C_{17}H_{34}$	1.22
17.583	Octadecane	$C_{18}H_{38}$	0.71
18.496	1,19-Eicosadiene	$C_{20}H_{38}$	0.27
18.562	1-Tricosene	$C_{23}H_{46}$	1.16
18.628	Nonadecane	$C_{19}H_{38}$	0.80
19.505	1,19-Eicosadiene	$C_{20}H_{38}$	0.20
19.565	Nonadecene	$C_{19}H_{38}$	0.98
19.624	Nonadecane	$C_{19}H_{40}$	0.61
20.467	1,19-Eicosadiene	$C_{20}H_{38}$	0.23
20.522	1-Tricosene	$C_{23}H_{46}$	0.95
20.576	Heneicosane	$C_{21}H_{44}$	0.79
21.440	5-Eicosene	$C_{21}H_{42}$	0.86
21.489	Docosane	$C_{22}H_{44}$	0.73
22.319	1-Tricosene	$C_{23}H_{46}$	0.79
22.363	Heneicosane	$C_{21}H_{44}$	0.71

23.163	1-Tetracosene	C ₂₄ H ₄₈	0.71
23.203	Tetracosane	C ₂₄ H ₅₀	0.69
23.975	9-Tricosene	C ₂₃ H ₄₆	0.64
24.012	Octacosane	C ₂₈ H ₅₈	0.64
24.756	Hexacosene	C ₂₆ H ₅₂	0.67
24.789	Hexaoxane	C ₂₆ H ₅₄	0.65
25.511	1-Docosene	C ₂₂ H ₄₄	0.55
25.538	Eicosane, 1-iodo	C ₂₀ H ₄₄	0.62
26.238	Eicosyl trifluoroacetate	C ₂₂ H ₄₁ F ₃ O ₂	0.46
26.262	Hexa cosine-1Iodo	C ₂₆ H ₅₁ I	0.60
26.962	Carbonic acid, octadecyl vinyl ester	C ₂₁ H ₄₀ O ₃	0.92
27.636	Carbonic acid, eicosyl vinyl ester	C ₂₃ H ₄₄ O ₃	0.80
28.290	Carbonic acid, eicosyl vinyl ester	C ₂₃ H ₄₄ O ₃	0.62
28.947	1-Octadecene	C ₁₈ H ₃₆	0.51

Table S2. GCMS result of oil sample with 10% fly ash (P- 500-FA-10)

Retention time	Compound name	Formulae	Area%
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2.626	Heptane	C_7H_{16}	0.41
2.849	Cyclohexene,4-methyl	C_7H_{12}	0.23
2.911	Cyclohexane, methyl	C_7H_{14}	0.21
3.069	Cyclohexene, 3- methyl	C_7H_{14}	0.41
3.226	Cyclopentene, 3-ethyl-	C_7H_{12}	0.24
3.377	Toluene	C_8H_{10}	1.36
3.418	Cyclohexene, 1-methy	C_7H_{14}	0.38
3.542	Ethylidenecyclobutane	C_8H_{12}	0.21
3.561	1,3-Cycloheptadiene	C_7H_{10}	0.25
3.653	1-Octene	C_8H_{16}	1.75
3.771	Octane	C_8H_{18}	0.61
4.693	Ethylbenzene	C_8H_{10}	0.37
4.828	p-Xylene	C_8H_{10}	0.63
4.991	Octadiene	$C_{18}H_{34}$	0.29
5.133	Nonene	C_9H_{18}	2.07
5.185	Nonane	C_9H_{20}	0.66
5.480	Cyclohexane, Propyl	C_9H_{18}	0.24
6.612	1,9-Decadiene	$C_{10}H_{81}$	0.24
6.751	1-Decene	$C_{10}H_{20}$	2.64
6.891	Decane	$C_{10}H_{22}$	0.64
8.227	Cycloundecene	$C_{10}H_{22}$	0.37

8.361	1-Undecene	$C_{11}H_{22}$	2.57
8.492	Undecane	$C_{11}H_{24}$	0.83
9.775	Cyclododecene	$C_{12}H_{24}$	0.40
9.899	Dodecene	$C_{12}H_{24}$	2.37
11.022	Dodecane	$C_{12}H_{26}$	0.82
11.239	1,12-Tridecadyne	$C_{13}H_{24}$	0.52
11.354	1-Tridecene	$C_{13}H_{26}$	2.13
11.467	Tridecane	$C_{13}H_{28}$	0.82
12.621	Tetradecadyne	$C_{14}H_{26}$	0.49
12.725	Tetradecene	$C_{14}H_{28}$	2.22
12.829	Nonadecene	$C_{19}H_{38}$	0.81
13.925	Cyclopentadecanol	$C_{15}H_{30}O$	0.41
14.020	1-Pentadecene	$C_{15}H_{30}$	1.97
14.114	Pentadecane	$C_{15}H_{32}$	0.78
15.158	Hexadecadyne	$C_{16}H_{34}$	0.37
15.245	Nonadecene	$C_{19}H_{38}$	1.70
15.331	Hexadecane	$C_{16}H_{32}$	0.79
16.327	Elcosadiene	$C_{20}H_{38}$	0.33
16.406	1-Heptadecene	$C_{17}H_{34}$	1.47
16.486	Heptadecane	$C_{17}H_{36}$	0.65
17.438	1,19-Icosadiene	$C_{20}H_{38}$	0.29
17.511	Octadecene	$C_{18}H_{36}$	1.30
17.581	Octadecane	$C_{18}H_{38}$	0.67

18.495	18-Nonadecene-1-ol	C ₁₉ H ₃₈ O	0.29
18.562	Nonadecene	C ₁₉ H ₃₈	1.20
18.627	Nonadecane	C ₁₉ H ₄₀	0.73
19.503	1-19, Icosadiene	C ₂₀ H ₃₈	0.20
19.564	3-IcoScene	C ₂₀ H ₄₀	0.98
19.623	Eicosane	C ₂₀ H ₄₂	0.53
20.467	1,19-Eicosadiene	C ₂₀ H ₄₀	0.19
20.522	Heneicos-1-ene	C ₂₁ H ₄₂	0.93
20.576	Henecosane	C ₂₁ H ₄₄	0.69
21.440	pentacosene	C ₂₅ H ₅₀	0.82
21.489	Heneicosane	C ₂₁ H ₄₄	0.62
22.319	1-Tricosene	C ₂₃ H ₄₆	0.74
22.363	Octacosane	C ₂₈ H ₅₈	0.60
23.163	1-Tricosene	C ₂₃ H ₄₆	0.66
23.205	Tetracosane	C ₂₃ H ₄₈	0.57
23.975	Octadecyl trifluoroacetate	C ₂₀ H ₃₇ F ₃ O ₂	0.70
24.011	Tertracosane,1-Iodo	C ₂₄ H ₄₇ I	0.53
24.757	1-Tricosene	C ₂₃ H ₂₆	0.59
24.789	Tetracosane,1-iodo	C ₂₄ H ₄₇ I	0.53
25.511	Cyclotetra cosane	C ₂₄ H ₄₈	0.49
25.540	Hexadecane-1 Iodo	C ₂₆ H ₅₁ I	0.48
26.239	1-Heptacosanol	C ₂₇ H ₅₄ O	0.38

26.262	Heptadecane	C ₂₇ H ₅₆	0.48
26.957	Eicosane	C ₂₀ H ₄₂	0.74
27.636	Carbonic acid, eicosyl vinyl ester	C ₂₃ H ₄₄ O ₃	0.62
28.287	Carbonic acid, eicosyl vinyl ester	C ₂₃ H ₄₄ O ₃	0.49
28.947	Carbonic acid, eicosyl vinyl ester	C ₂₃ H ₄₄ O ₃	0.40

Table S3. GCMS result of oil sample with 15% fly ash (P- 500-FA-15)

Retention time	Compound name	formulae	Area%
2.626	Heptane	C ₇ H ₁₆	0.51
2.849	Cyclohexene,3- methyl	C ₇ H ₁₄	0.26
2.911	Cyclohexane, methyl	C ₇ H ₁₄	0.23
3.069	Cyclohexene, 4- methyl	C ₇ H ₁₂	0.46
3.226	Cyclopentene, 3- ethyl-	C ₇ H ₁₂	0.26
3.376	Toluene	C ₇ H ₈	1.50
3.419	Cyclohexene, 1- methy	C ₇ H ₁₄	0.41

3.542	Cyclooctene	C ₈ H ₁₆	0.22
3.654	1-Octene	C ₈ H ₁₆	1.90
3.771	Octane	C ₈ H ₁₈	0.67
4.693	Ethylbenzene	C ₈ H ₁₀	0.40
4.828	p-Xylene	C ₈ H ₁₀	0.67
4.991	1,8-Nonadiene	C ₉ H ₁₆	0.31
5.134	1-Nonene	C ₉ H ₁₈	2.20
5.185	p-Xylene	C ₈ H ₁₀	0.46
5.269	Nonane	C ₉ H ₁₈	0.69
6.612	1,9-Decadiene	C ₁₀ H ₁₈	0.33
6.751	1-Decene	C ₁₀ H ₂₀	2.73
6.891	Decane	C ₁₀ H ₂₂	0.66
8.227	Undecadiene	C ₁₁ H ₂₀	0.38
8.360	1-Undecene	C ₁₁ H ₂₂	2.65
8.493	Undecane	C ₁₁ H ₂₄	0.85
9.775	1,11-Dodecadiene	C ₁₂ H ₂₂	0.40
9.899	1-Dodecene	C ₁₂ H ₂₄	2.33
10.022	Dodecane	C ₁₂ H ₂₆	0.89
11.239	1,13-Tetradecadiene	C ₁₄ H ₂₆	0.49
11.352	1-Tridecene	C ₁₃ H ₂₆	2.10
11.467	Tridecane	C ₁₃ H ₂₈	0.80
12.620	1-13 tetradecadien,	C ₁₄ H ₂₆	0.47
12.725	2-Tetradecene,	C ₁₄ H ₂₈	2.16

12.829	Tetradecane	$C_{14}H_{30}$	0.79
13.925	1,13-Tetradecadiene	$C_{14}H_{28}$	0.40
14.020	Pentadecene	$C_{15}H_{30}$	1.94
14.115	Pentadecane	$C_{15}H_{32}$	0.77
15.158	1,13-Tetradecadiene	$C_{14}H_{26}$	0.37
15.246	1-Octadecenel	$C_{18}H_{36}O$	1.69
15.331	Hexadecane	$C_{16}H_{34}$	0.81
16.327	1,15 hexadecanol	$C_{16}H_{32}O$	0.33
16.407	Heptadecene	$C_{17}H_{34}$	1.49
16.486	Heptadecane	$C_{17}H_{36}$	0.65
17.439	1,19-EiCosadiene	$C_{20}H_{38}$	0.30
17.511	1-Nonadecene	$C_{19}H_{38}$	1.34
17.583	Octadecane	$C_{18}H_{38}$	0.69
18.496	1,19-Eicosadiene	$C_{20}H_{38}$	0.30
18.563	Nonadecene	$C_{19}H_{38}$	1.24
18.628	Nonadecane	$C_{19}H_{40}$	0.80
19.505	1,19-Eicosadiene	$C_{20}H_{40}$	0.20
19.565	Nonadecene	$C_{19}H_{38}$	1.03
19.626	Eicosane	$C_{20}H_{42}$	0.56
20.467	1,19-Eicosadiene	$C_{20}H_{38}$	0.23
20.523	Nona decene	$C_{19}H_{38}$	0.98
20.578	Heneicosane	$C_{21}H_{42}$	0.73
21.440	Docosene	$C_{22}H_{44}$	0.86

21.490	Docosane	$C_{22}H_{46}$	0.66
22.319	1-Tricosene	$C_{23}H_{46}$	0.78
22.363	Hexadecane	$C_{16}H_{34}$	0.64
23.163	Henicosanol	$C_{21}H_{42}O$	0.68
23.203	Tetra cosane	$C_{24}H_{50}$	0.59
23.975	Heptadecyl flourobutarate	$C_{20}H_{33}F_7O_2$	0.61
24.012	Penta cosane	$C_{25}H_{52}$	0.57
24.756	Hexaoxane	$C_{26}H_{54}$	0.59
24.757	Hexacosene	$C_{26}H_{52}$.59
24.789	Eicosane -1 Iodo	$C_{20}H_{39}I$	0.54
25.511	Hexacosene	$C_{26}H_{52}$	0.49
25.538	Hexadecane-1Iodo	$C_{16}H_{31}I$	0.53
26.238	Eicosyl trifluoroacetate	$C_{22}H_{41}F_3O_2$	0.46
26.262	Eicosane	$C_{20}H_{42}$	0.91
26.962	Heptadecene	$C_{17}H_{34}$	0.77
27.636	Eicosane	$C_{20}H_{42}$	0.62
28.292	Carbonic acid Eicosyl vinyl ester	$C_{23}H_{44}O_3$	0.51

-Table S4. GCMS result of oil sample with 20% fly ash (P- 500-FA-20)

Retention time	Compound name	Formulae	Area %
2.627	Heptane	C ₇ H ₁₆	0.70
2.848	Cyclohexene,3 methyl	C ₈ H ₁₂	0.22
2.912	Cyclohexane, methyl	C ₇ H ₁₄	0.25
3.069	Cyclohexene, 3- methyl	C ₇ H ₁₆	0.28
3.226	Cyclopentene, 3- ethyl	C ₇ H ₁₂	0.21
3.376	Toluene	C ₇ H ₈	0.47
3.418	Cyclohexene, 1- methyl	C ₇ H ₁₄	0.36
3.653	1-Octene	C ₈ H ₁₆	1.59
3.770	Octane	C ₈ H ₁₈	0.85
4.825	p-Xylene	C ₈ H ₁₀	0.40
5.132	1-Nonen	C ₉ H ₁₈	1.89
5.268	Nonane	C ₉ H ₂₀	0.88
6.611	1,9-Decadiene	C ₁₀ H ₁₈	0.17
6.750	1-Decene	C ₁₀ H ₂₀	2.45
6.890	Decane	C ₁₀ H ₂₂	0.91
8.226	1,10-Undecadiene	C ₁₁ H ₂₀	0.26
8.359	5-Undecene	C ₁₁ H ₂₂	2.36
8.492	Undecane	C ₁₁ H ₂₄	1.11

9.774	Cyclododecene	$C_{11}H_{20}$	0.31
9.897	1-Dodecene	$C_{12}H_{24}$	2.12
10.021	Dodecane	$C_{12}H_{26}$	1.14
11.237	Cyclododecene	$C_{12}H_{24}$	0.38
11.351	1-Tridecene	$C_{13}H_{26}$	2.00
11.465	Tridecane	$C_{13}H_{28}$	1.10
12.620	1,13-Tetradecadiene	$C_{14}H_{26}$	0.36
12.724	2-Tetradecene	$C_{14}H_{28}$	2.09
12.828	Tetradecane	$C_{14}H_{30}$	1.09
13.924	1,12-Tridecadiene	$C_{13}H_{24}$	0.30
14.019	1-Pentadecene	$C_{15}H_{30}$	1.85
14.114	Pentadecane	$C_{15}H_{32}$	1.08
15.157	1,15-Pentadecanediol	$C_{15}H_{32}O$	0.28
15.244	7-Hexadecene	$C_{16}H_{32}$	1.64
15.331	Hexadecane	$C_{16}H_{34}$	1.12
16.326	1,19-Eicosadiene	$C_{20}H_{38}$	0.25
16.406	1-Heptadecene	$C_{17}H_{34}$	1.42
16.486	Heptadecane	$C_{17}H_{36}$	0.94
17.437	1,19-Eicosadiene	$C_{20}H_{40}$	0.21
17.511	1-Nonadecene	$C_{19}H_{38}$	1.30
17.582	Tetradecane	$C_{18}H_{38}$	0.97
18.562	1-Nonadecene	$C_{19}H_{38}$	1.20
18.628	Nonadecane	$C_{19}H_{40}$	1.07

19.565	5-Eicosene	C ₂₀ H ₄₀	0.98
19.625	Eicosane	C ₂₀ H ₄₂	0.82
20.522	Henicos-1-ene	C ₂₁ H ₄₂	0.93
20.578	Hen eicosane	C ₂₁ H ₄₄	1.03
21.441	5-Eicosene,	C ₂₀ H ₄₀	0.80
21.490	Docosane	C ₂₂ H ₄₆	0.94
22.319	1-Tricosene	C ₂₃ H ₄₆	0.72
22.364	TTetradecane,4 ethyl	C ₁₆ H ₃₄	0.90
23.164	3-Eicosene	C ₂₀ H ₄₀	0.64
23.205	Eicosane	C ₂₀ H ₄₂	0.87
23.976	1-Heneicosanol	C ₂₁ H ₄₂ O	0.62
24.013	Tetradecane, 1-iodo	C ₁₄ H ₂₉ I	0.80
24.759	Tricosene	C ₂₃ H ₄₆	0.54
24.791	Hexa decane- Iodo-	C ₁₆ H ₃₁ I	0.78
25.514	Heptacos-1-ene	C ₂₇ H ₅₄	0.41
25.539	Hexadecane-1Iodo	C ₁₆ H ₃₁ I	0.75
26.264	Eicosane	C ₂₀ H ₄₂	1.06
27.640	Sulfurous acid, butyl heptadecyl.	C ₂₁ H ₄₄ O ₃ S	0.78
28.295	Eicosane	C ₂₀ H ₄₂	0.61
28.951	Carbonic acid, eicosyl vinyl ester	C ₂₃ H ₄₄ O ₃	0.49

NMR results of Pyrolysis oil of waste plastic with 20% fly ash catalyst.

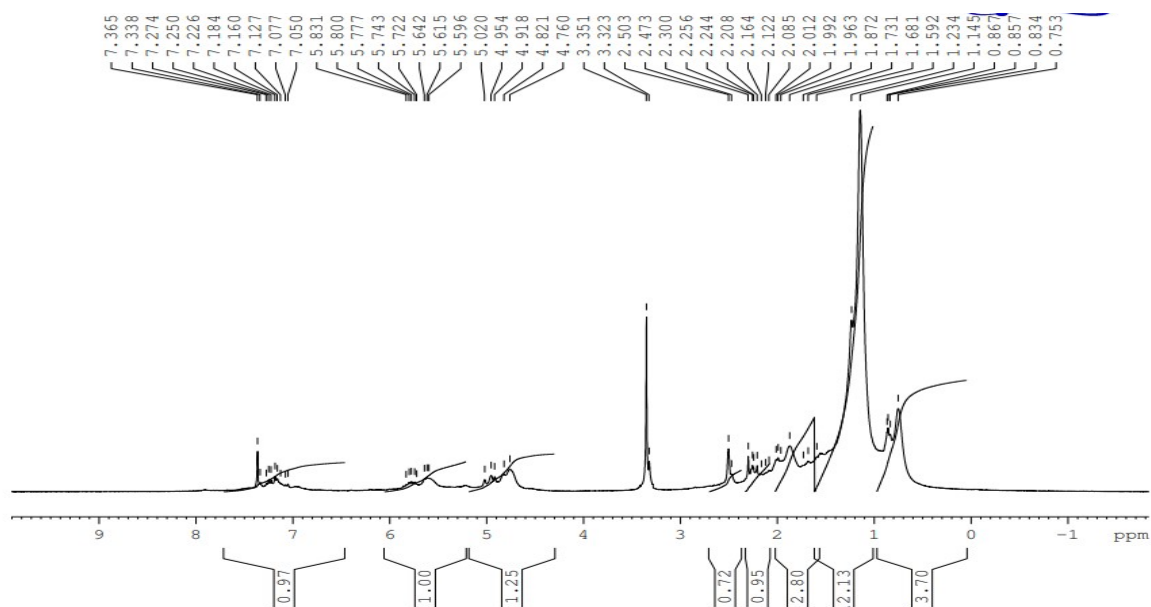


Figure S1 ^1H NMR analyses of liquid product with 20% fly ash samples

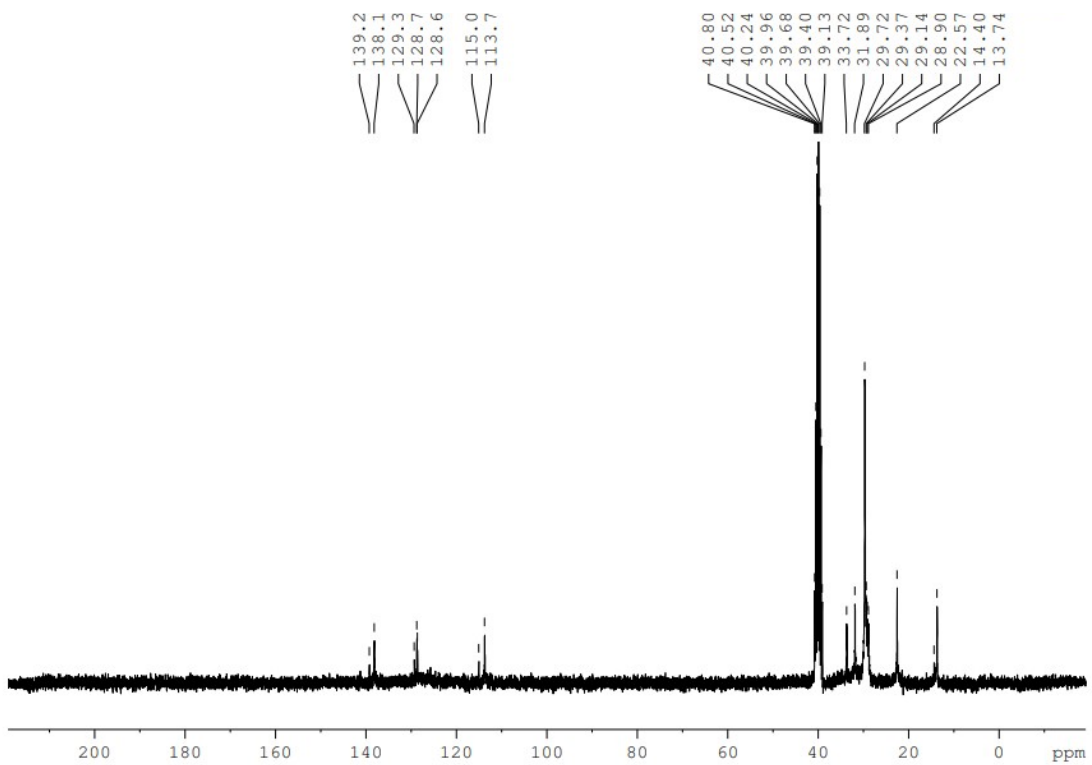


Figure S2. ^{13}C NMR analyses of liquid product with 20% fly ash samples