# Supplementary Materials: Study on the Catalytic Pyrolysis Mechanism of Lignite by using Extracts as Model Compounds

**Jianwei Liu, Qian Zhang, Litong Liang and Wei Huang**

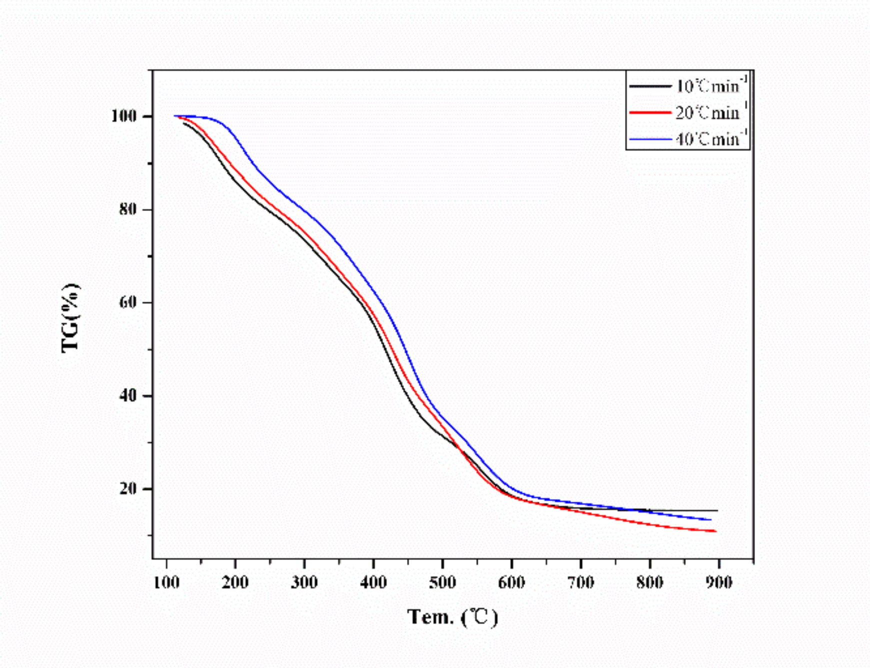


**Figure S1.** TGA curves for EX-Fe(N) at different heating rates

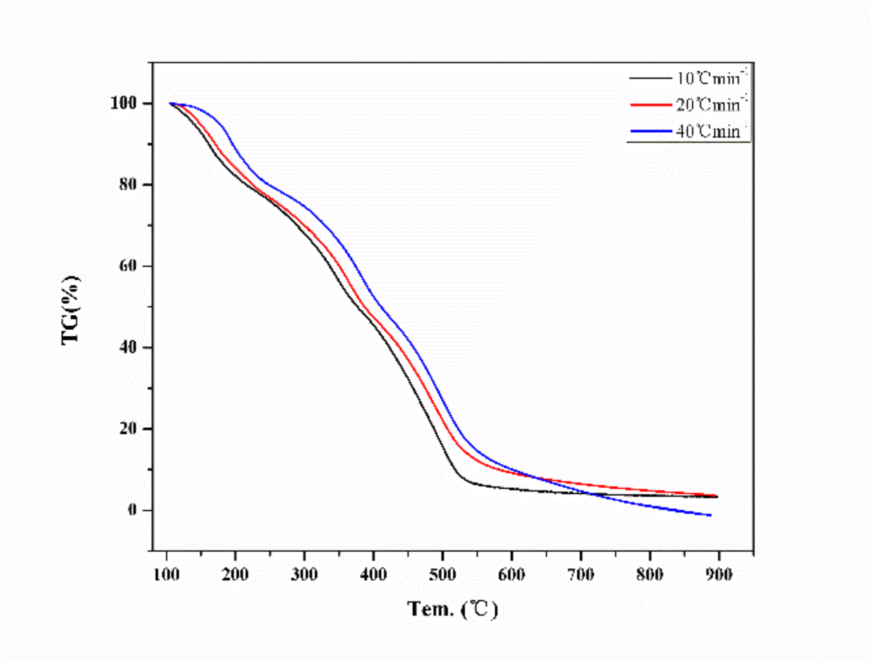


**Figure S2.** TGA curves for EX-Fe(C) at different heating rates

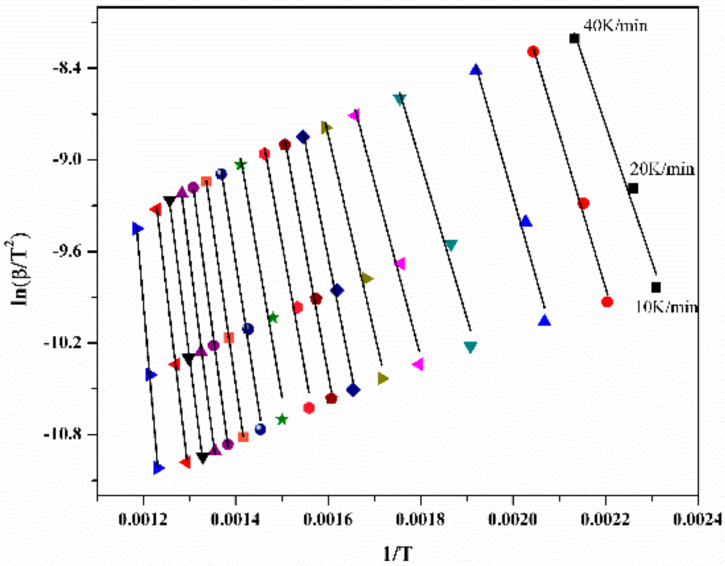


**Figure S3.** Arrhenius plot of DAEM method for EX-Fe(N)

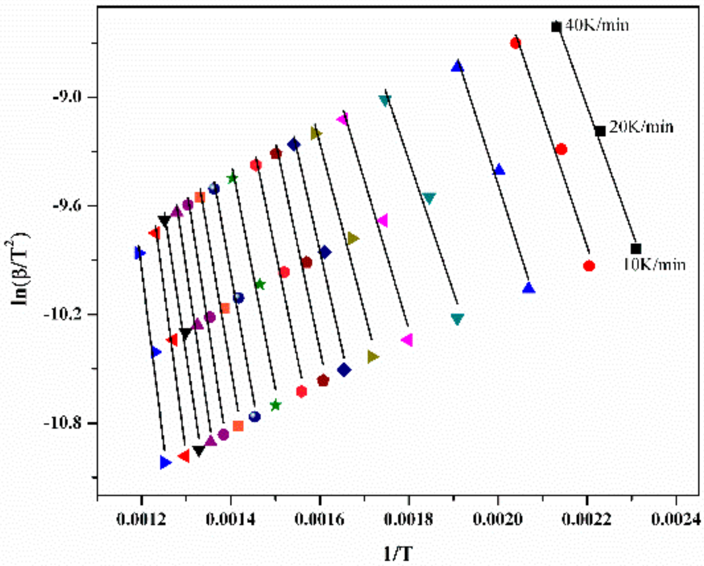


**Figure S4.** Arrhenius plot of DAEM method for EX-Fe(C)

**Table S1.** Typical components in THF extract detected by GC×GC-MS

| Blob ID | Compound Name | Retention I (min) | Retention II (sec) | Peak Volume | Percent Response |
|---|---|---|---|---|---|
| 1 | Dimethyl sulfone | 6.59 | 2.53 | 5.54E+04 | 0.78 |
| 2 | Pentanoic acid | 7.79 | 1.10 | 1.45E+04 | 0.20 |
| 3 | Acetic acid, butyl ester | 9.39 | 1.10 | 1.85E+04 | 0.26 |
| 4 | Propanoic acid, 2-methoxy- | 9.29 | 1.87 | 3.06E+04 | 0.43 |
| 5 | 2-Hexanol, 2-methyl- | 10.09 | 1.48 | 3.89E+05 | 5.48 |
| 6 | 2-Cyclopenten-1-one, 2-hydroxy-3-methyl- | 12.39 | 1.98 | 4.09E+04 | 0.58 |
| 7 | Phenol | 16.29 | 1.87 | 4.46E+04 | 0.63 |
| 8 | xylene | 18.59 | 1.32 | 1.12E+05 | 1.58 |
| 9 | 2-Butanone, 4,4-dimethoxy- | 23.49 | 1.92 | 2.97E+04 | 0.42 |
| 10 | 1-Octene | 21.19 | 1.26 | 2.31E+04 | 0.33 |
| 11 | Heptane, 3-ethyl- | 22.79 | 1.32 | 9.35E+03 | 0.13 |
| 12 | p-Cresol | 20.99 | 1.98 | 2.36E+04 | 0.33 |
| 13 | Benzaldehyde dimethyl acetal | 23.29 | 1.76 | 4.80E+04 | 0.68 |
| 14 | Ethanone, 1-(1-cyclohexen-1-yl)- | 21.79 | 2.14 | 6.30E+04 | 0.89 |
| 15 | Octanoic acid | 25.69 | 1.37 | 2.83E+04 | 0.40 |
| 16 | Catechol | 26.69 | 2.36 | 3.67E+04 | 0.52 |
| 17 | Naphthalene | 27.09 | 2.25 | 5.31E+04 | 0.75 |
| 18 | Benzaldehyde, 3-hydroxy- | 31.29 | 2.91 | 2.30E+04 | 0.32 |
| 19 | Naphthalene, 1-methyl- | 32.39 | 2.20 | 3.00E+04 | 0.42 |
| 20 | Caprolactam | 28.39 | 4.29 | 2.08E+05 | 2.93 |
| 21 | Benzaldehyde, 4-hydroxy- | 33.59 | 3.13 | 6.16E+05 | 8.68 |
| 22 | Benzaldehyde, 3-hydroxy-4-methoxy- | 35.59 | 3.13 | 5.54E+05 | 7.81 |

| | | | | | |
|---|---|---|---|---|---|
| 23 | Homovanillyl alcohol | 36.69 | 2.47 | 8.24E+04 | 1.16 |
| 24 | Benzoic acid, 4-(isopropyl)oxy-, methyl ester | 37.89 | 2.91 | 6.44E+04 | 0.91 |
| 25 | 1-Hexene, 3,5-dimethyl- | 39.89 | 1.37 | 6.86E+05 | 9.67 |
| 26 | Heptanal, 2-methyl- | 41.79 | 1.10 | 7.14E+04 | 1.01 |
| 27 | Dodecanoic acid | 43.09 | 1.43 | 5.44E+04 | 0.77 |
| 28 | 4-Undecene, 10-methyl-, (E)- | 43.99 | 1.37 | 2.53E+04 | 0.36 |
| 29 | Naphthalene, 1,2-dimethyl- | 38.09 | 2.20 | 3.92E+04 | 0.55 |
| 30 | Acetophenone, 4'-hydroxy- | 37.09 | 3.19 | 4.42E+04 | 0.62 |
| 31 | Cadina-1(10),6,8-triene | 44.79 | 1.81 | 1.98E+05 | 2.79 |
| 32 | 3-Eicosene, (E)- | 47.79 | 1.43 | 1.45E+05 | 2.04 |
| 33 | Ethanol, 2-(dodecyloxy)- | 49.19 | 1.48 | 2.04E+05 | 2.88 |
| 34 | 6-Isopropyl-1,4-dimethylnaphthalene | 48.09 | 2.09 | 1.01E+06 | 14.18 |
| 35 | Undecanal, 2-methyl- | 49.29 | 1.15 | 1.42E+05 | 2.00 |
| 36 | 1-Octanamine, n-octyl- | 51.09 | 1.26 | 2.00E+05 | 2.81 |
| 37 | 2-Pentadecanone, 6,10,14-trimethyl- | 53.79 | 1.32 | 1.83E+05 | 2.59 |
| 38 | Heptadecane, 2,6-dimethyl- | 56.09 | 1.10 | 8.96E+04 | 1.26 |
| 39 | Tridecane, 6-cyclohexyl- | 57.99 | 1.21 | 6.16E+04 | 0.87 |
| 40 | Fluorene | 44.39 | 2.69 | 2.13E+04 | 0.30 |
| 41 | Benzaldehyde, 4-hydroxy-3,5-dimethoxy- | 45.79 | 3.52 | 1.20E+05 | 1.70 |
| 42 | Naphthalene, 1,6-dimethyl-4-(1-methylethyl)- | 48.49 | 2.03 | 2.58E+04 | 0.36 |
| 43 | Anthracene | 51.69 | 3.19 | 1.94E+05 | 2.74 |

| | | | | | |
|---|---|---|---|---|---|
| 44 | 1,2-Benzenedicarboxylic acid, butyl 2-methylpropyl ester | 53.89 | 2.25 | 2.72E+05 | 3.83 |
| 45 | Phthalic acid, butyl hexyl ester | 56.99 | 2.36 | 3.28E+05 | 4.62 |
| 46 | Anthracene, 2-methyl- | 55.79 | 3.08 | 2.42E+04 | 0.34 |
| 47 | Ethanone, 1-(3-hydroxy-4-methoxyphenyl)- | 39.39 | 3.08 | 4.95E+04 | 0.70 |
| 48 | Phenanthrene, 3-methyl- | 56.49 | 3.19 | 3.48E+04 | 0.49 |
| 49 | Phenanthrene, 2,3-dimethyl- | 60.19 | 3.02 | 8.88E+04 | 1.25 |
| 50 | Pyrene | 60.99 | 3.57 | 2.98E+04 | 0.42 |
| 51 | 1-Dodecanol, 2-hexyl- | 61.59 | 1.21 | 1.13E+05 | 1.60 |
| 52 | Fluoranthene | 63.09 | 3.74 | 4.71E+04 | 0.66 |
| 53 | Heptadecane, 2,3,5-trimethyl- | 64.16 | 1.52 | 7.32E+04 | 1.02 |
| 54 | Nonadecane, 2-methyl | 65.48 | 1.81 | 4.28E+04 | 1.49 |
| 55 | Eicosane, 3-methyl | 67.34 | 1.79 | 9.47E+04 | 1.35 |

**Table S2.** Variation of E and A obtained from DAEM method for different samples

| α | EX | | | EX-Fe(N) | | | EX-Fe(C) | | |
|---|---|---|---|---|---|---|---|---|---|
| | E(kJ/mol) | A($min^{-1}$) | $R^2$ | E(kJ/mol) | A($min^{-1}$) | $R^2$ | E(kJ/mol) | A($min^{-1}$) | $R^2$ |
| 0.1 | 74.31 | 1.02E+03 | 0.9642 | 54.16 | 8.75E+00 | 0.9909 | 56.75 | 2.41E+01 | 0.9789 |
| 0.15 | 83.64 | 2.98E+03 | 0.9884 | 60.12 | 2.04E+01 | 0.9251 | 60.76 | 3.44E+01 | 0.9463 |
| 0.2 | 88.63 | 4.35E+03 | 0.9643 | 67.34 | 1.82E+02 | 0.9712 | 63.55 | 4.18E+01 | 0.9662 |
| 0.25 | 84.65 | 1.70E+04 | 0.9523 | 71.49 | 5.85E+02 | 0.9621 | 65.47 | 6.68E+01 | 0.9283 |
| 0.3 | 94.95 | 1.84E+04 | 0.9671 | 82.56 | 7.06E+02 | 0.9523 | 68.42 | 8.63E+01 | 0.9333 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 0.35 | 108.06 | 3.68E+04 | 0.9649 | 89.81 | 1.44E+04 | 0.9468 | 77.34 | 1.43E+02 | 0.9115 |
| 0.4 | 125.51 | 8.47E+04 | 0.9877 | 99.62 | 3.58E+04 | 0.9001 | 90.25 | 1.81E+02 | 0.9541 |
| 0.45 | 136.05 | 2.75E+05 | 0.9898 | 108.91 | 5.53E+04 | 0.9016 | 95.88 | 3.31E+02 | 0.9277 |
| 0.5 | 139.06 | 1.05E+05 | 0.9579 | 123.52 | 2.57E+05 | 0.9324 | 98.89 | 3.19E+02 | 0.9406 |
| 0.55 | 146.03 | 8.51E+05 | 0.9196 | 135.69 | 9.59E+05 | 0.9303 | 105.22 | 4.97E+02 | 0.9295 |
| 0.6 | 159.99 | 1.15E+06 | 0.9841 | 143.97 | 4.79E+06 | 0.9318 | 113.23 | 1.10E+03 | 0.9619 |
| 0.65 | 173.82 | 5.49E+06 | 0.9959 | 149.14 | 5.69E+06 | 0.9713 | 119.79 | 2.08E+03 | 0.9317 |
| 0.7 | 188.13 | 2.76E+07 | 0.9985 | 155.32 | 1.79E+08 | 0.9948 | 130.37 | 7.67E+03 | 0.9584 |
| 0.75 | 196.74 | 1.52E+08 | 0.9956 | 168.73 | 2.34E+08 | 0.9765 | 136.46 | 1.32E+04 | 0.9663 |
| 0.8 | 197.42 | 1.66E+08 | 0.9955 | 175.34 | 3.30E+08 | 0.9841 | 144.39 | 4.95E+04 | 0.9629 |
| 0.85 | 209.76 | 6.03E+08 | 0.9984 | 182.44 | 3.76E+08 | 0.9998 | 152.65 | 6.61E+04 | 0.9558 |
| 0.9 | 286.03 | 1.28E+09 | 0.9978 | 208.75 | 6.64E+09 | 0.8935 | 161.17 | 1.06E+05 | 0.9444 |