

Supplementary Material
for
Characterization and Contaminant Assessment of Waste Tire Char Produced
in an Industrial-Scale Auger Reactor

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Table S1. Qualitative chromatographic analysis of char - compounds with a content above 1% by area

RT	Compound	RI lit	RI exp	Area	%
35.09	Tetradecane	1400	1400	1144897	1.22
39.43	Pentadecane	1500	1500	1305020	1.39
43.54	Heksadecane	1600	1600	1808428	1.92
47.44	Heptadecane	1700	1700	2184241	2.32
51.15	Octadecane	1800	1800	1768524	1.88
54.69	Nonadecane	1900	1900	1750004	1.86
58.07	Icosane	2000	2000	1987063	2.11
61.30	Heneicosane	2100	2100	1526087	1.62
61.48	Pyrene	2113	2106	1281461	1.36
62.84	Trimethylphenanthrene isomer		2150	1238409	1.32
64.39	Docosane	2200	2200	2144599	2.28
67.36	Tricosane	2300	2300	1777833	1.89
70.21	Tetracosane	2400	2400	1589635	1.69
72.96	Pentacosane	2500	2500	1480336	1.57
75.60	Heksacosane	2600	2600	2314549	2.46
78.15	Heptacosane	2700	2700	1383121	1.47
80.62	Octacosane	2800	2800	1599652	1.70
83.00	Nonacosane	2900	2900	1776787	1.89
85.31	Triacontane	3000	3000	1548324	1.65
87.54	Hentriacontane	3100	3100	1753930	1.87
89.70	Dotriacontane	3200	3200	2306661	2.45
90.54	Anthanthrene		3240	1271192	1.35
91.81	Tritriacontane	3300	3300	2183725	2.32
93.85	Tetratriacontane	3400	3400	2102658	2.24
95.83	Pentatriacontane	3500	3500	2669888	2.84
97.76	Hexatriacontane	3600	3600	2166419	2.30
98.20	Tris(2,4-di-tert-butylphenyl) phosphate	3582	3623	6549923	6.97
99.70	Heptatriacontane	3700	3700	2079679	2.21
101.87	Octatriacontane	3800	3800	1391979	1.48
104.34	Nonatriacontane	3900	3900	1487290	1.58
107.21	Tetracontane	4000	4000	1150573	1.22

Table S2. Qualitative chromatographic analysis of char - compounds with a content of up to 1.0% by area

RT	Compound	RI lit	RI exp	Area	%
40.50	1,4,5-Trimethylnaphthalene	1515	1526	621069	0.66
47.82	Biphenyl isomer		1710	650789	0.69
56.94	2-Phenylnaphthalene	1968	1967	507973	0.54
60.89	2-Benzylnaphthalene		2087	519928	0.55
64.77	Retene	2198	2213	663053	0.71
65.92	2-Methylpyrene	2253	2252	601916	0.64
69.10	cis-11-Eicosenoic acid	2360	2361	574936	0.61
71.43	Benz[a]anthracene	2441	2444	540675	0.58
74.92	2-methylchrysene/9-Methylbenz[a]anthracene	2580	2574	923940	0.98
75.91	8-Methylbenz[a]anthracene		2612	475418	0.51
77.08	benzo[cd]pyrenone isomer (MW=254)		2658	488202	0.52
81.34	1,12-Dimethylbenz[a]anthracene	2822	2830	572389	0.61
81.56	Benzo(a)pyrene	2840	2839	795642	0.85
84.89	n-methylbenzo(a)pyrene (MW=266)		2982	759443	0.81

Table S3. Qualitative chromatographic analysis of char - compounds with a content of up to 0.5% by area

RT	Compound	RI lit	RI exp	Area	%
5.30	Octane	800	800	345151	0.37
39.25	Trimethyltetradecane		1496	375856	0.40
43.32	Naphthalene isomer		1595	445823	0.47
49.59	Biphenyl isomer		1758	347988	0.37
50.96	1-Methyl-9,10-dihydrophenanthrene	1795	1795	430894	0.46
52.67	Biphenyl isomer		1843	439896	0.47
54.27	2-Methylphenanthrene	1890	1888	479639	0.51
54.75	1-Methylphenanthrene	1900	1902	371302	0.40
55.12	3-Methylphenanthrene	1909	1913	478492	0.51
56.83	1-Methylanthracene		1963	406514	0.43
58.97	3,6-Dimethylphenanthrene	2027	2028	352928	0.38

59.37	1,7-Dimethylphenanthrene	2051	2040	428363	0.46
62.55	Trimethylphenanthrene isomer		2140	405648	0.43
63.74	Hydrocarbon isomer		2179	418457	0.45
65.25	4-Methylpyrene	2232	2229	405798	0.43
71.73	Chrysene	2445	2455	389105	0.41
74.64	5-methylchrysene	2577	2564	381133	0.41
76.47	7-Methylbenz[a]anthracene		2634	367191	0.39
79.79	Benzo(k)fluoranthene		2766	376869	0.40
81.86	Perylene		2852	438830	0.47
84.40	n-methylbenzo(a)pyrene (MW=266)		2961	465164	0.49
84.54	n-methylbenzo(a)pyrene (MW=266)		2967	449048	0.48
88.20	Indeno(1,2,3,c,d)pyrene		3131	427287	0.45

Table S4. Qualitative chromatographic analysis of char - compounds with a content of up to 0.35% by area

RT	Compound	RI lit	RI exp	Area	%
35.69	1,7-Dimethylnaphthalene	1414	1414	218352	0.23
35.82	1,3-Dimethylnaphthalene	1417	1417	260492	0.28
37.80	Tetradecane, 4,11-dimethyl-	1462	1462	268006	0.29
39.02	4-Methylbiphenyl	1492	1491	299692	0.32
41.15	Trimethylnaphthalene isomer		1542	233561	0.25
41.28	Trimethylnaphthalene isomer		1545	231625	0.25
41.85	1,6,7-Trimethylnaphthalene	1568	1559	210911	0.22
45.86	Hydrocarbon isomer		1659	197655	0.21
44.51	3-Ethylbiphenyl	1628	1625	296944	0.32
49.07	1,2,3,4-Tetrahydrophenanthrene	1738	1744	272301	0.29
49.44	Biphenyl isomer		1754	262364	0.28
50.11	Phenanthrene	1775	1772	225455	0.24
51.50	Dihydrophenanthrene isomer		1810	329144	0.35
51.96	Dihydrophenanthrene isomer		1823	276225	0.29
53.40	Biphenyl isomer		1864	315406	0.34
54.45	2-Methylantracene	1896	1893	326694	0.35
55.29	2-Methylantracene	1918	1918	194204	0.21
58.38	2,5-Dimethylphenanthrene	2009	2010	306415	0.33
58.79	2,7-Dimethylantracene	2009	2022	301652	0.32

59.20	2,7-Dimethylphenanthrene	2028	2035	297226	0.32
59.73	Fluoranthene	2054	2051	273534	0.29
60.66	1-Benzyl-naphthalene		2080	270152	0.29
64.51	Benzo[a]fluorene		2204	333293	0.35
66.15	1-Methylpyrene	2257	2259	199386	0.21
66.55	1-Chloroeicosane	2264	2273	199165	0.21
68.81	Dimethylpyrene isomer (MW=230)		2351	221119	0.24
69.36	Dimethylpyrene isomer (MW=230)		2370	286580	0.30
69.56	Dimethylpyrene isomer (MW=230)		2377	304832	0.32
69.76	Dimethylpyrene isomer (MW=230)		2384	224459	0.24
70.44	2-styrylnaphthalene	2410	2408	274347	0.29
72.41	PAH isomer (MW=244)		2480	206405	0.22
74.45	3-methylchrysene	2565	2556	253492	0.27
78.60	1,12-Dimethylbenzo[c]phenanthrene		2718	217414	0.23
79.31	n,n-Dimethylbenzo[c]phenanthrene (MW=256)		2747	293512	0.31
79.74	Benzo(b)fluoranthene		2764	279881	0.30
82.42	Benzo(e)pyrene		2876	264221	0.28
83.73	n-methylbenzo(a)pyrene (MW=266)		2932	328297	0.35
89.45	Benzo(g,h,i)perylene		3188	218693	0.23

Table S5. Qualitative chromatographic analysis of char - compounds with a content of up to 0.35% by area

RT	Compound	RI lit	RI exp	Area	%
35.69	1,7-Dimethylnaphthalene	1414	1414	218352	0.23
35.82	1,3-Dimethylnaphthalene	1417	1417	260492	0.28
37.80	Tetradecane, 4,11-dimethyl-	1462	1462	268006	0.29
39.02	4-Methylbiphenyl	1492	1491	299692	0.32
41.15	Trimethylnaphthalene isomer		1542	233561	0.25
41.28	Trimethylnaphthalene isomer		1545	231625	0.25
41.85	1,6,7-Trimethylnaphthalene	1568	1559	210911	0.22
45.86	Hydrocarbon isomer		1659	197655	0.21
44.51	3-Ethylbiphenyl	1628	1625	296944	0.32
49.07	1,2,3,4-Tetrahydrophenanthrene	1738	1744	272301	0.29
49.44	Biphenyl isomer		1754	262364	0.28
50.11	Phenanthrene	1775	1772	225455	0.24
51.50	Dihydrophenanthrene isomer		1810	329144	0.35
51.96	Dihydrophenanthrene isomer		1823	276225	0.29

53.40	Biphenyl isomer		1864	315406	0.34
54.45	2-Methylanthracene	1896	1893	326694	0.35
55.29	2-Methylanthracene	1918	1918	194204	0.21
58.38	2,5-Dimethylphenanthrene	2009	2010	306415	0.33
58.79	2,7-Dimethylanthracene	2009	2022	301652	0.32
59.20	2,7-Dimethylphenanthrene	2028	2035	297226	0.32
59.73	Fluoranthene	2054	2051	273534	0.29
60.66	1-Benzyl naphthalene		2080	270152	0.29
64.51	Benzo[a]fluorene		2204	333293	0.35
66.15	1-Methylpyrene	2257	2259	199386	0.21
66.55	1-Chloroeicosane	2264	2273	199165	0.21
68.81	Dimethylpyrene isomer (MW=230)		2351	221119	0.24
69.36	Dimethylpyrene isomer (MW=230)		2370	286580	0.30
69.56	Dimethylpyrene isomer (MW=230)		2377	304832	0.32
69.76	Dimethylpyrene isomer (MW=230)		2384	224459	0.24
70.44	2-styryl naphthalene	2410	2408	274347	0.29
72.41	PAH isomer (MW=244)		2480	206405	0.22
74.45	3-methylchrysene	2565	2556	253492	0.27
78.60	1,12-Dimethylbenzo[c]phenanthrene		2718	217414	0.23
79.31	n,n-Dimethylbenzo[c]phenanthrene (MW=256)		2747	293512	0.31
79.74	Benzo(b)fluoranthene		2764	279881	0.30
82.42	Benzo(e)pyrene		2876	264221	0.28
83.73	n-methylbenzo(a)pyrene (MW=266)		2932	328297	0.35
89.45	Benzo(g,h,i)perylene		3188	218693	0.23

Table S6. Qualitative chromatographic analysis of WTP-char - compounds with a content of up to 0.1% by area

RT	Compound	RI lit	RI exp	Area	%
5.41	2-Hexanol	801	802	79447	0.08
5.59	5-Methyl-2-hexanol	815	807	40010	0.04
7.76	Ethylbenzene	855	856	15007	0.02
8.15	p-Xylene	865	865	19204	0.02
9.72	Nonane	900	900	15514	0.02
14.51	Benzene, 1,2,4-trimethyl-	990	990	26086	0.03
15.05	Decane	1000	1000	25098	0.03
16.67	Benzene, cyclopropyl-	1032	1030	15322	0.02
17.70	o-Propyltoluene	1047	1049	12605	0.01

17.93	1-Phenylbutane	1054	1053	14461	0.02
18.16	Decane, 2,6,7-trimethyl-	1058	1058	60430	0.06
19.15	2-Ethyl-p-xylene	1074	1076	35889	0.04
19.48	p-Cymenene	1090	1082	45450	0.05
20.45	Undecane	1100	1100	21849	0.02
22.21	Indan, 5-methyl-	1136	1134	52607	0.06
22.77	Indan, 4-methyl-	1145	1145	63292	0.07
23.31	n-Pentylbenzene	1157	1155	35683	0.04
24.45	Naphthalene	1182	1178	19994	0.02
24.76	1,6-Dimethylindan	1174	1184	34488	0.04
24.84	2,2-Dimethylindane	1181	1185	17401	0.02
25.26	Benzene, 1-methyl-4-(1-methyl-2-propenyl)-	1191	1193	40776	0.04
26.31	Undecane, 2,6-dimethyl-	1210	1214	42552	0.05
26.56	Cyclopentylbenzene	1212	1219	14691	0.02
27.12	1-Methyltetralin	1229	1231	34284	0.04
27.84	4,6-Dimethylindan	1235	1246	63328	0.07
28.75	2-Methyldodecane	1264	1264	61173	0.07
29.36	4,7-Dimethylindan	1282	1277	60094	0.06
31.59	1,8-Dimethyltetralin	1318	1324	60559	0.06
31.71	Hydrocarbon isomer		1327	85699	0.09
32.49	6-Ethyltetraline	1339	1343	62140	0.07
32.87	6-Methyltridecane	1344	1352	53016	0.06
33.36	Heptylbenzene	1368	1362	71013	0.08
35.25	Hydrocarbon isomer		1404	75937	0.08
35.50	Hydrocarbon isomer		1409	72036	0.08
36.55	2,3-Dimethylnaphthalene	1440	1434	50539	0.05
37.40	2,6,10-Trimethyltridecane	1449	1453	84455	0.09
38.17	Tetradecane, 6,9-dimethyl-		1471	89256	0.09
38.45	Acenaphthene	1486	1477	43031	0.05
38.91	Tetradecane, 2,5-dimethyl-	1483	1488	41937	0.04
39.80	Trimethylnaphthalene isomer		1509	12986	0.01
40.08	2,5-Di-tert-butylphenol	1514	1516	84544	0.09
40.31	2,3,6-Trimethylnaphthalene	1515	1521	78158	0.08
41.46	2,6,10-Trimethyltetradecane	1555	1549	91697	0.10
43.83	Hydrocarbon isomer		1607	94487	0.10
45.19	4-Ethylbiphenyl	1654	1642	95622	0.10
50.49	Anthracene	1782	1782	57449	0.06
51.77	anthracene, 1,2-dihydro-10-methyl-	1813	1818	98167	0.10

78.29	n,n-Dimethylbenzo[c]phenanthrene (MW=256)		2706	80205	0.09
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