

Electronic Supplementary Information (ESI)

**Fate of Pyrene on Mineral Surfaces during Thermal Remediation as a Function of  
Temperature**

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Environmental Science: Processes and Impacts

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## 1. GC/MS Methods

### *Extracts –*

Injection Volume: 1 uL

Inlet Temperature: 320 °C

Column Flow: 1.2 mL/min

Temperature Program:

	Rate (°C/min)	Final Temperature (°C)	Hold Time (min)
Initial		50	0.4
Ramp 1	25	195	1.5
Ramp 2	8	255	0
Ramp 3	2.5	260	0
Ramp 4	20	295	0
Ramp 5	10	310	3.5

MSD Transfer Line Temperature: 300 °C

MS Source Temperature: 250 °C

MS Quad Temperature: 150 °C

### *Headspace –*

Injection Volume: 200 uL

Inlet Temperature: 250 °C

Column Flow: 0.7 mL/min

Split Ratio: 20:1

Temperature Program:

	Rate (°C/min)	Final Temperature (°C)	Hold Time (min)
Initial		35	5
Ramp 1	25	250	2

MSD Transfer Line Temperature: 300 °C

MS Source Temperature: 230 °C

MS Quad Temperature: 150 °C

## 2. Parent Removal Experiments

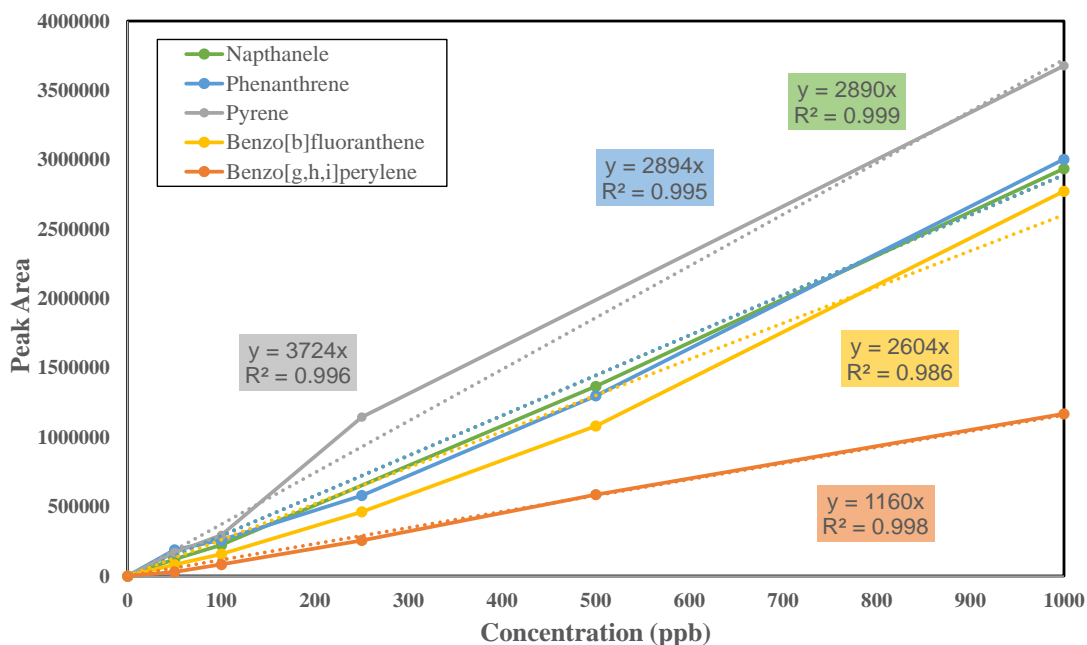
**Table S1:** p-value from ANOVA of treatment temperature and percent removal of pyrene in parent removal experiments. p-values < 0.05 are highlighted in green.

p-value	Dry	Wet
Bir	3.6E-05	0.0010
Mag	0.00011	0.20
Hem	0.0067	0.043

**Table S2:** Lowest significant difference (LSD) calculated from ANOVA of treatment temperature and percent removal of pyrene in parent removal experiments. Differences in removal greater than LSD are highlighted in green.

Experiment	LSD	AVG <sub>150</sub>	$\Delta_{150-200}$	AVG <sub>200</sub>	$\Delta_{200-250}$	AVG <sub>250</sub>	$\Delta_{150-250}$	
Dry	Bir	8.1	46.8	25.2	72.0	28.0	100.0	53.2
	Mag	5.2	46.7	16.9	63.6	11.0	74.6	27.8
	Hem	17.7	19.2	14.2	33.4	36.9	70.3	51.1
	LSD	AVG <sub>75</sub>	$\Delta_{75-100}$	AVG <sub>100</sub>	$\Delta_{100-150}$	AVG <sub>150</sub>	$\Delta_{75-150}$	
Wet	Bir	8.8	60.1	19.5	79.5	12.1	91.6	31.6
	Mag	19.9	60.4	18.1	78.5	-1.1	77.4	17.0
	Hem	12.1	65.5	10.5	75.9	9.5	85.5	20.0

### 3. Mineral-Limited Experiments



**Figure S1:** Standard curves derived from MassHunter qualitative analysis.

**Table S3:** Detected by-products from dry, mineral-limited experiments with magnetite listed by temperature with match score, molecular weight, and peak area. Estimated masses are included for compounds included in calibration curve (Figure S1).

Temperature	Compound	Score	MW	Peak Area	Mass ( $\mu\text{g}$ )
500 °C	4,5-diethyl-octane	97	170.2	26277377	
	5,6-dimethyl-decane	96	170.2	21254399	
	5-methyl-undecane	91	170.2	4170193	
	3-ethyl-5-methyl-1-propyl-cyclohexane	89	168.2	7704961	
	(1,2-dimethylbutyl)-cyclohexane	92	168.2	16568368	
	Undecyl-cyclohexane	81	238.3	8400050	
	Octyl-cyclohexane	91	196.2	13062669	
	Naphthalene	96	128.1	38510240	40
	Phenanthrene	98	178.1	2645088	2.7
	Benzo[a]fluorene	87	216.1	262814	
	1-methyl-pyrene	93	216.1	1478264	
	Perylene	82	252.1	107528	
	1-phenyl-pyrene	97	278.1	5311060	
	Benzo[ghi]perylene	91	276.1	181424	0.21
Indeno[1,2,3-cd]pyrene	84	276.1	102196		
300 °C	9-ethenyl-anthracene	96	204.1	6861137	
	Fluoranthene	94	202.1	12437093	10
200 °C	2,2',5,5'-tetramethyl-1,1'-Biphenyl	82	210	76709	
	Cyclopenta[def]phenanthrene	94	190	1286791	
	1-phenyl-naphthalene	85	204	9648460	
	Benzo[a]fluorene	90	216	614798	
	Benzo[c]fluorene	87	216	230230	
100 °C	Cyclopenta[def]phenanthrene	95	190.1	1259038	
	4,5-dihydro-acephenanthrylene	91	204.1	10143710	
	Benzo[c]fluorene	86	216.1	55594	
	Benzo[b]fluorene	94	216.1	534719	
	Benzo[a]fluorene	83	216.1	196969	

**Table S4:** Detected by-products from saturated, mineral-limited experiments with magnetite listed by temperature with match score, molecular weight, and peak area. Estimated masses are included for compounds included in calibration curve (Figure S1).

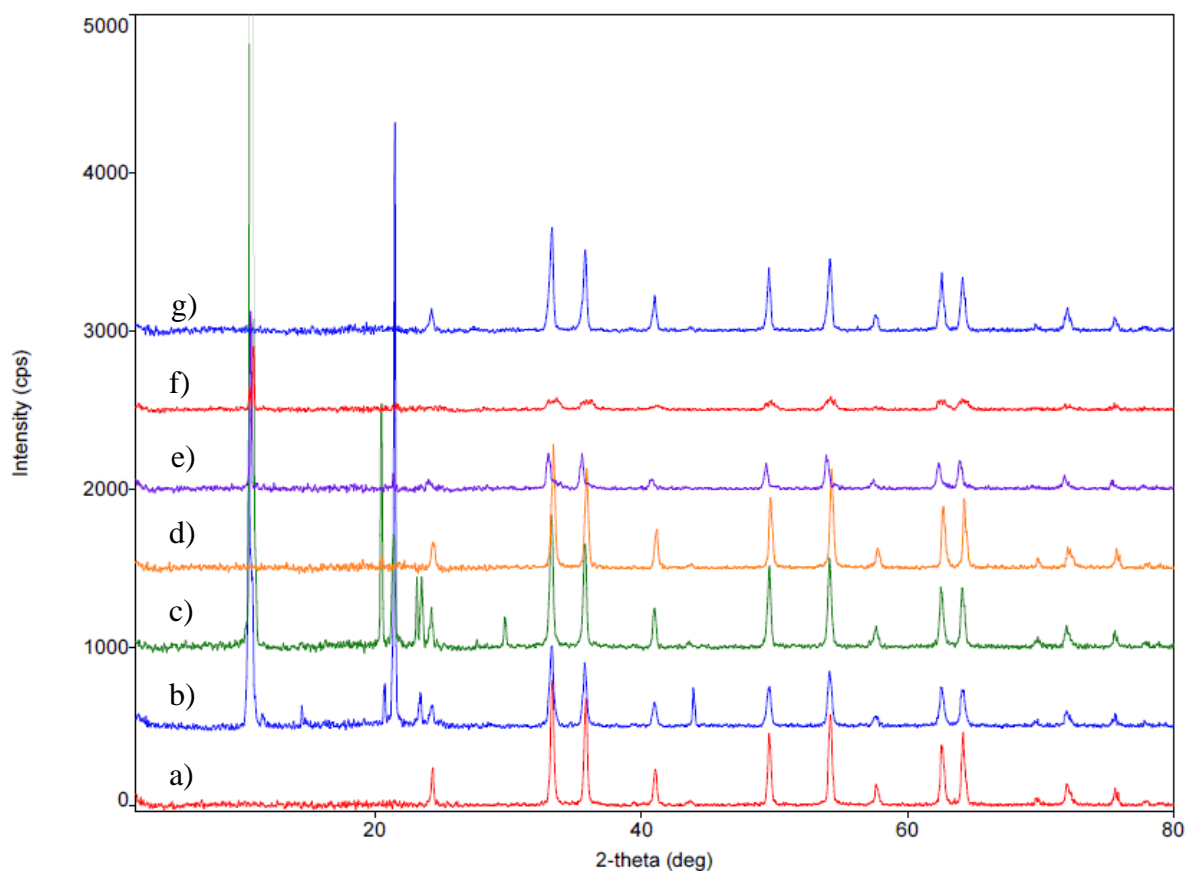
<i>Temperature</i>	<i>Compound</i>	<i>Score</i>	<i>MW</i>	<i>Peak Area</i>	<i>Mass (µg)</i>
<b>500 °C</b>	3-n-Propyl-5-methylhexan-2-one	92	156.2	6431370	
	4,5-diethyl-octane	97	170.2	27918984	
	5,6-dimethyl-decane	95	170.2	22753803	
	5-methyl-undecane	91	170.2	4489649	
	3-ethyl-5-methyl-1-propyl-cyclohexane	89	168.2	8005084	
	(1,2-dimethylbutyl)-cyclohexane	92	168.2	16709801	
	Octyl-cyclohexane	90	196.2	13264257	
	Cyclohexaneethanol	83	128.1	3569167	
	3-Hexanone	84	100.1	23292995	
	Biphenyl	82	154.1	98833	
	5,8-Tridecadiene	82	212.2	968078	
	Naphtho[2,1-b]furan	81	168.1	43112	
	Dibenzofuran	89	168.1	146441	
	Benzophenone	95	182.1	224426	
	<b>Phenanthrene</b>	<b>99</b>	<b>178.1</b>	<b>7489250</b>	<b>7.8</b>
	1-(phenylmethylene)-indene	95	204.1	162821	
	Phenalen-1-one	90	180.1	8025703	
	Cyclopenta(def)phenanthrenone	82	204.1	3417633	
	Benzanthrene	91	216.1	409789	
	Benzo[a]fluorene	94	216.1	3172901	
	1-methyl-pyrene	95	216.1	10474807	
	3,4-dihydro-cyclopenta(cd)pyrene	89	228.1	284082	
	Naphtho[2,1,8,7-klmn]xanthene	82	242.1	469916	
	5-Methoxy-benzo[c]phenanthrene	82	258.1	5580678	
	1-hydroxypyrene	87	218.1	3464928	
	<b>Benzo[e]pyrene</b>	<b>95</b>	<b>252.1</b>	<b>901841</b>	<b>1.0</b>
1-phenyl-pyrene	97	278.1	30292897		
Pentacene	90	278.1	1181447		
<b>Indeno[1,2,3-cd]pyrene</b>	<b>94</b>	<b>276.1</b>	<b>355826</b>	<b>0.92</b>	
<b>300 °C</b>	4,4-dimethyl-undecane	80	184.2	67776	
	4,5-diethyl-octane	85	170.2	233128	
	3,4,5-trimethyl-heptane	91	142.2	139071	
	(1,2-dimethylbutyl)-cyclohexane	91	168.2	285668	
	(1-methylethyl)-cyclohexane	85	126.1	185384	
	3-n-Propyl-2,4-pentanedione	81	142.1	54900	
	Cyclopenta[def]phenanthrene	97	190.1	1453981	
	9-ethenyl-anthracene	90	204.1	10600039	
	Benzo[c]fluorene	93	216.1	659899	
	Benzo[a]fluorene	95	216.1	659912	
	1,3-dimethyl-pyrene	80	230.1	1403443	
	Isobutyl Stearate	92	340.3	9304170	
	1-Hydroxypyrene	84	218.1	194074	
<b>200 °C</b>	Cyclopenta[def]phenanthrene	96	190.1	778656	
	4,5-dihydro-acephenanthrylene	94	204.1	6637244	
	Benzo[a]fluorene	92	216.1	366328	
	Benzo[c]fluorene	90	216.1	136785	
<b>100 °C</b>	Cyclopenta[def]phenanthrene	96	190.1	872696	
	9-ethenyl-anthracene	90	204.1	7531669	
	Benzo[a]fluorene	92	216.1	425216	
	Benzanthrene	86	216.1	223624	

## 4. Mineral Analysis

**Table S5:** Specific surface area of selected minerals determined by N<sub>2</sub>-BET.

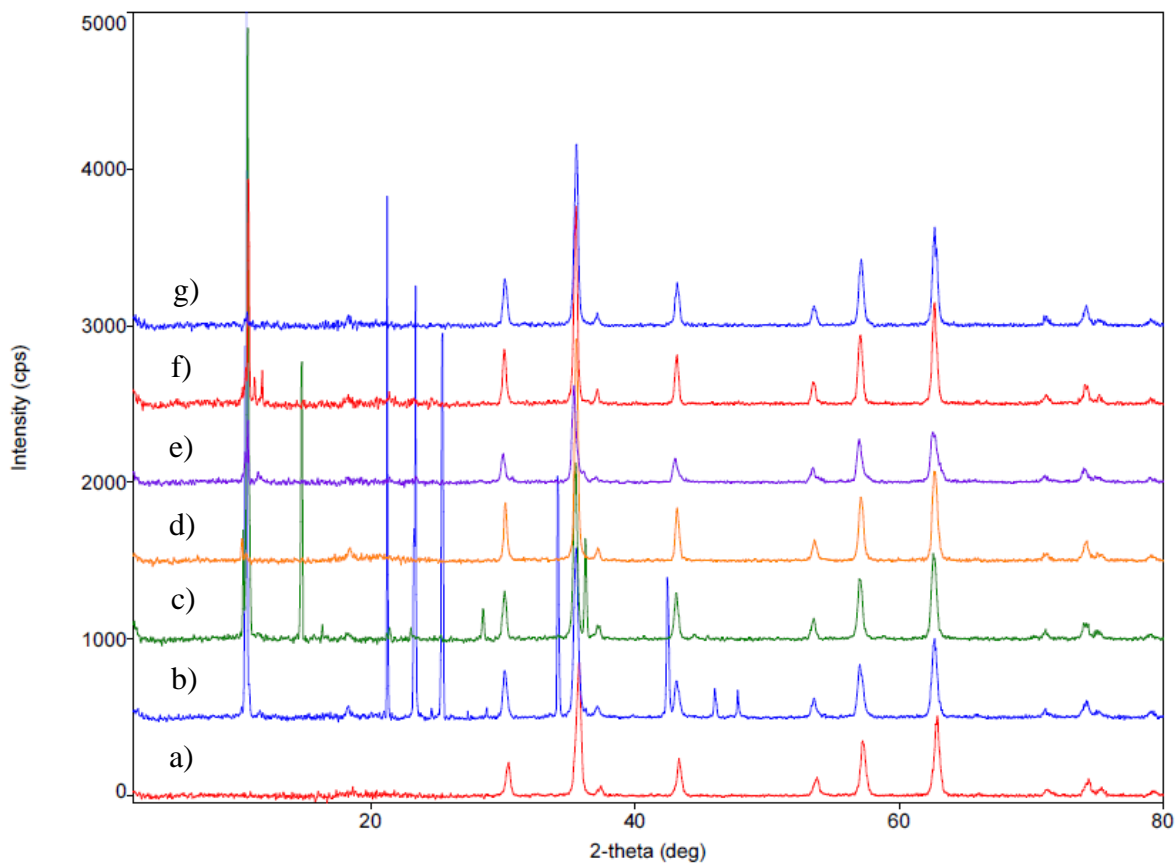
Mineral	Formula	Specific Surface Area (m <sup>2</sup> /g)
Birnessite	δ-MnO <sub>2</sub>	118
Magnetite	Fe <sub>3</sub> O <sub>4</sub>	5.7
Hematite	Fe <sub>2</sub> O <sub>3</sub>	7.4
Quartz	SiO <sub>2</sub>	3.7

### 4.1. XRD Patterns

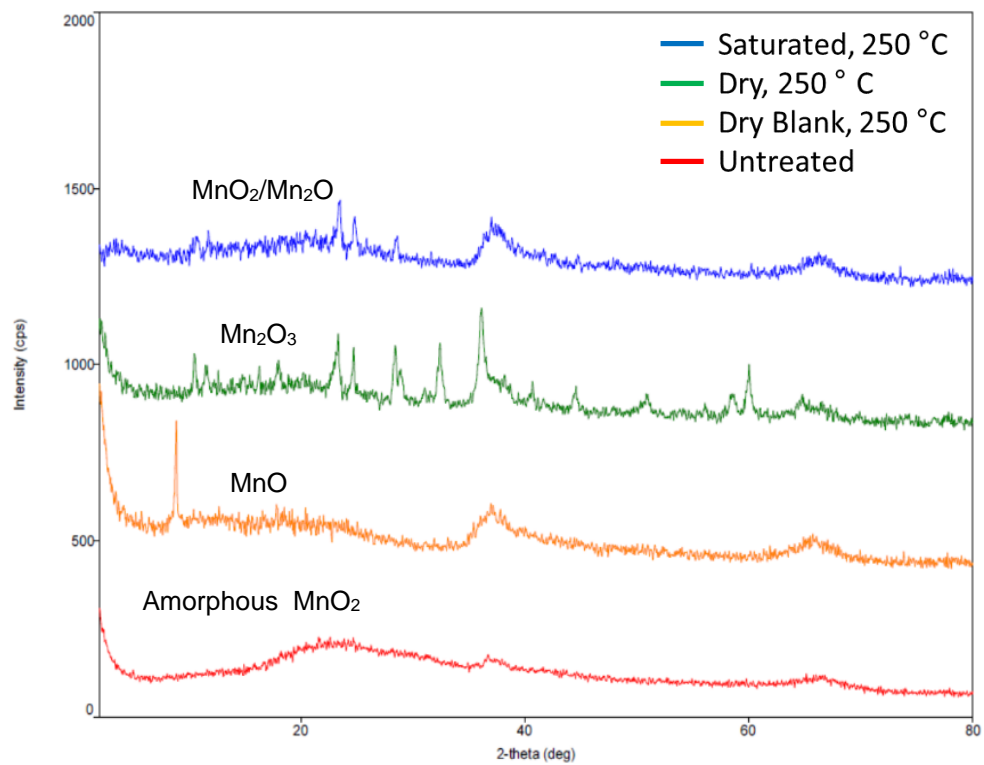


**Figure S2.** XRD patterns showing no bulk transformation of hematite under selected conditions: a) raw hematite, b) hematite treated at 150 °C for 30 min in air with 0.050 g pyrene and 50 uL of H<sub>2</sub>O, c) hematite treated at 150 °C for 30 min in N<sub>2</sub> with 0.050 g pyrene, d) hematite treated at 150 °C for 30 min in N<sub>2</sub> without pyrene, e) hematite treated at 250 °C for 30 min in air with 0.050 g pyrene and 50 uL of H<sub>2</sub>O, f) hematite treated at 250 °C for 30 min in N<sub>2</sub> with 0.050 g pyrene, g) hematite treated at 250 °C for 30 min in N<sub>2</sub> without pyrene



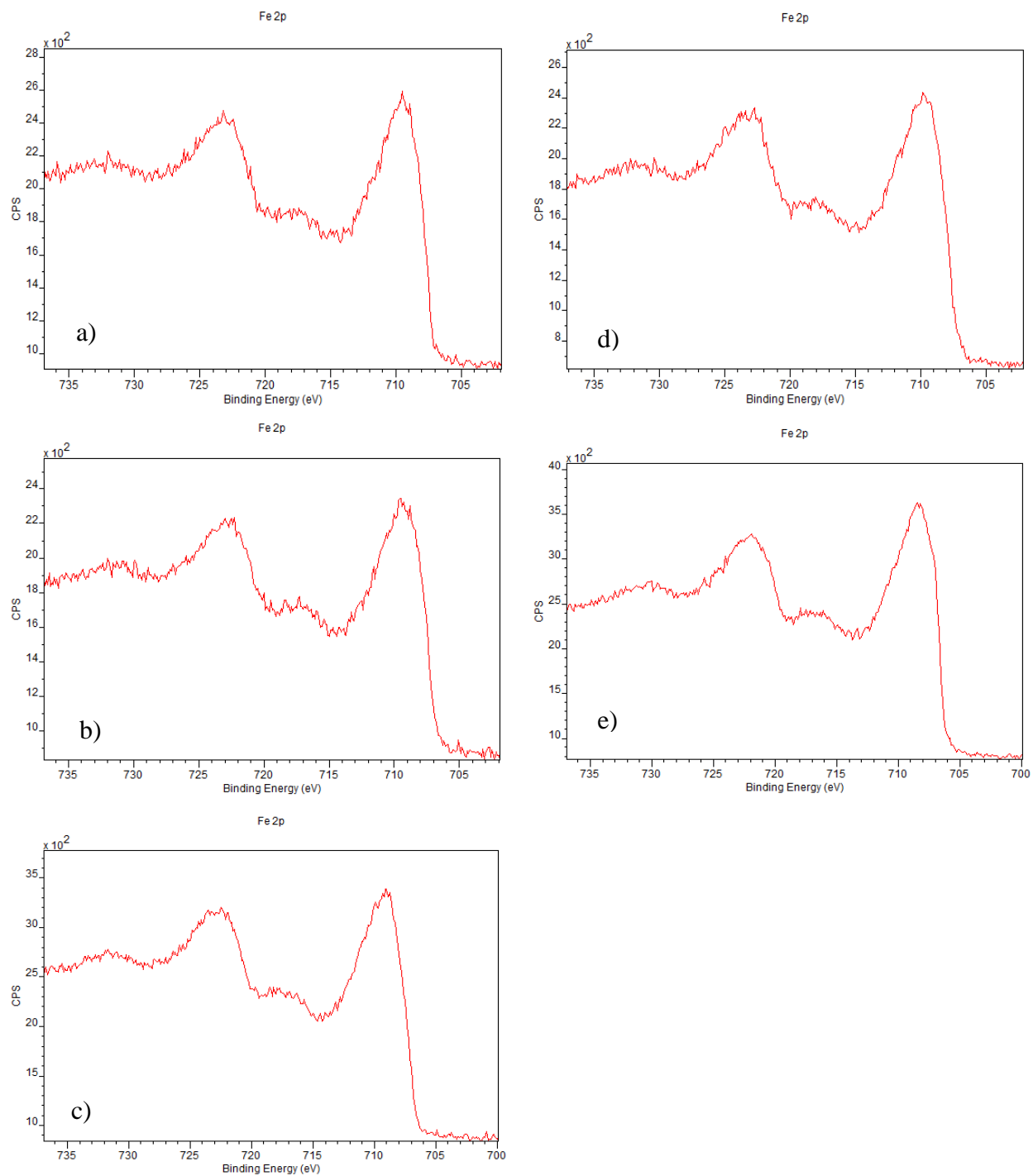


**Figure S3.** XRD patterns showing no bulk transformation of magnetite under various conditions: a) raw magnetite, b) magnetite treated at 150 °C for 30 min in air with 0.050 g pyrene and 50 uL of H<sub>2</sub>O, c) magnetite treated at 150 °C for 30 min in N<sub>2</sub> with 0.050 g pyrene, d) magnetite treated at 150 °C for 30 min in N<sub>2</sub> without pyrene, e) magnetite treated at 250 °C for 30 min in air with 0.050 g pyrene and 50 uL of H<sub>2</sub>O, f) magnetite treated at 250 °C for 30 min in N<sub>2</sub> with 0.050 g pyrene, g) magnetite treated at 250 °C for 30 min in N<sub>2</sub> without pyrene

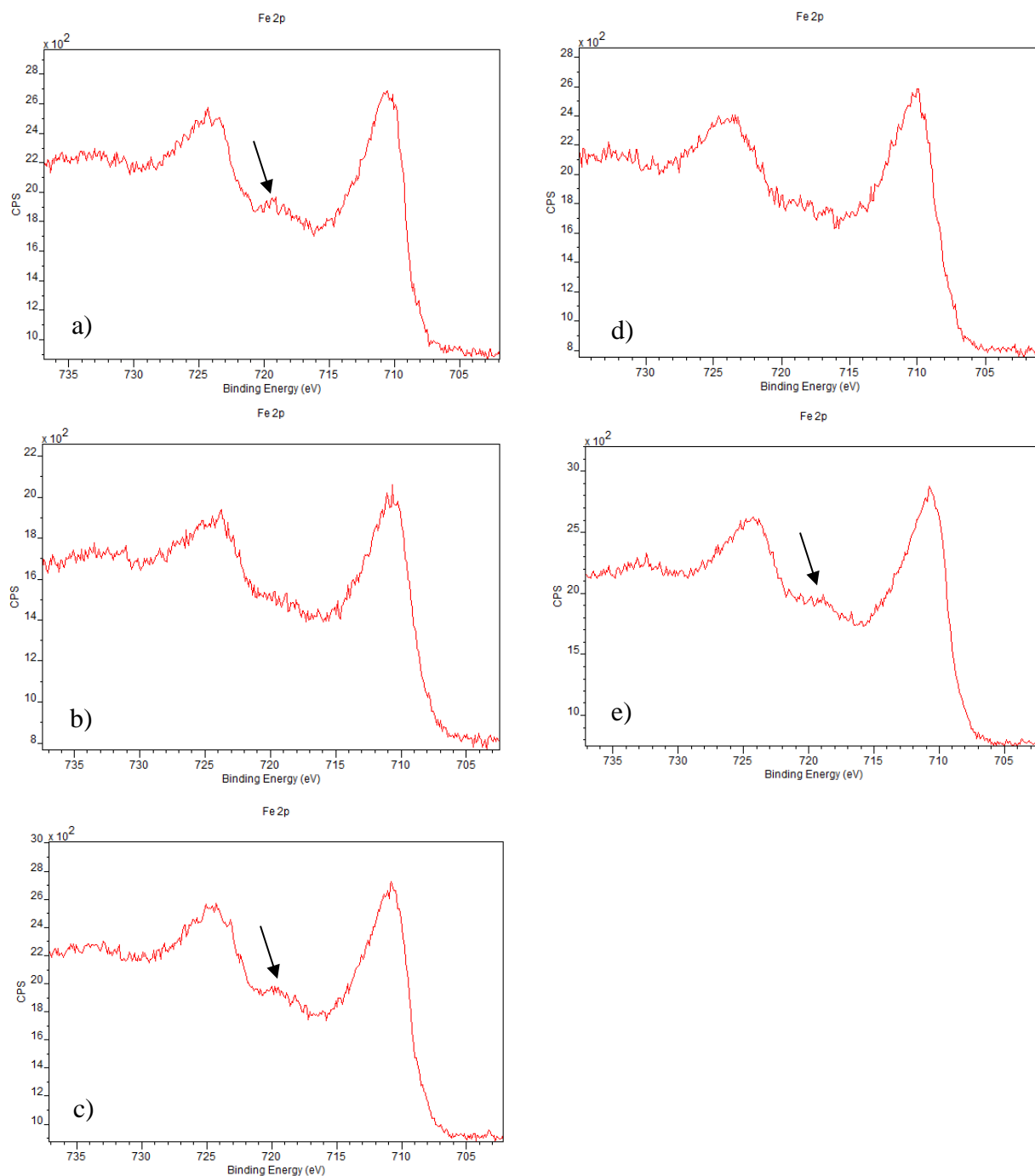


**Figure S4:** XRD patterns of birnessite after treatment under various conditions. Crystal phases detected shown next to diffraction patterns.

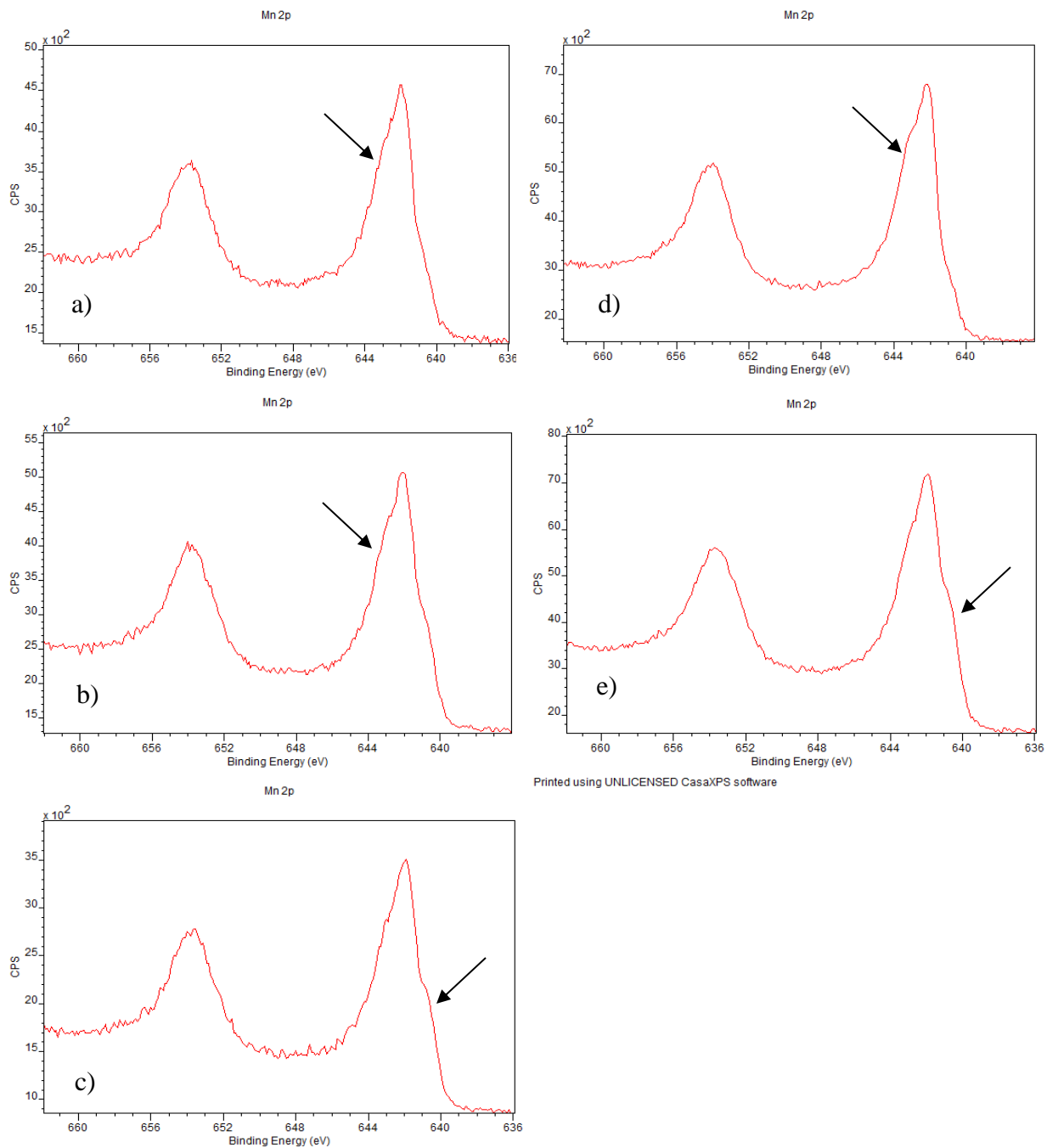
## 4.2. XPS Spectra



**Figure S5.** XPS Fe 2p spectra for a) untreated hematite, b) hematite treated at 250 °C for 30 min in N<sub>2</sub>, c) hematite treated at 250 °C for 30 min in air with 100 uL H<sub>2</sub>O, d) hematite treated at 250 °C for 30 min in N<sub>2</sub> with 0.050 g pyrene, e) hematite treated at 250 °C for 30 min in air with 0.050 g pyrene and 100 uL H<sub>2</sub>O,



**Figure S6.** XPS Fe 2p spectra for a) untreated magnetite, b) magnetite treated at 250 °C for 30 min in N<sub>2</sub>, c) magnetite treated at 250 °C for 30 min in air with 100  $\mu$ L H<sub>2</sub>O, d) magnetite treated at 250 °C for 30 min in N<sub>2</sub> with 0.050 g pyrene, e) magnetite treated at 250 °C for 30 min in air with 0.050 g pyrene and 100  $\mu$ L H<sub>2</sub>O. Satellite peak indicating presence of hematite indicated by arrows.



**Figure S7.** XPS Mn 2p spectra for a) untreated birnessite, b) birnessite treated at 250 °C for 30 min in N<sub>2</sub>, c) birnessite treated at 250 °C for 30 min in N<sub>2</sub> with 0.050 g pyrene, d) birnessite treated at 250 °C for 30 min in air with 100 uL H<sub>2</sub>O, e) birnessite treated at 250 °C for 30 min in air with 0.050 g pyrene and 100 uL H<sub>2</sub>O. Presence of shoulder indicated by arrows. Shoulder located on the left side of the peak indicates the presence of MnO<sub>2</sub>. Shoulder located on the right side of the peak indicates the presence of Mn<sub>2</sub>O<sub>3</sub>.

### 4.3. Electron transfer calculations

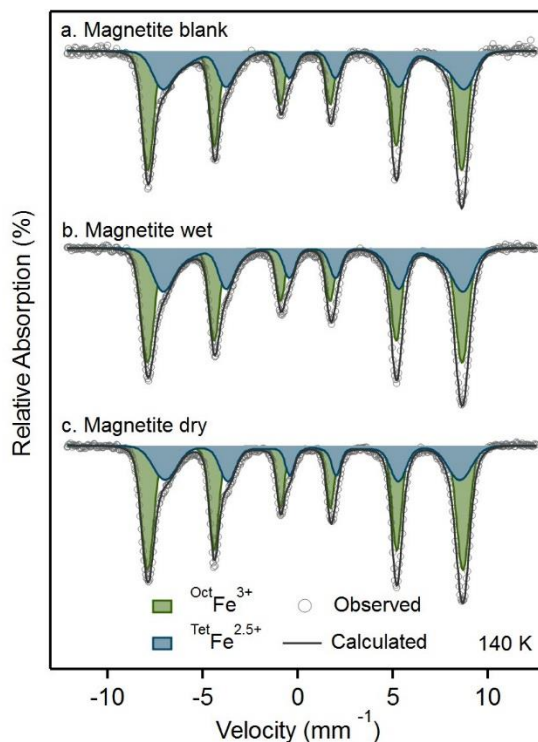
$$\begin{aligned}
 &C_{16}H_{10} + 6H^+ + 6e^- \rightarrow 8C_2H_2 \\
 &2(Fe_2^{3+}Fe^{2+})O_4 + H_2O \rightarrow 3Fe_2O_3 + 2H^+ + 2e^- \\
 &C_{16}H_{10} + 6(Fe_2^{3+}Fe^{2+})O_4 + 3H_2O \rightarrow 9Fe_2O_3 + 8C_2H_2 \\
 \text{Mass of } F_3O_4 &= (0.05 \text{ g pyrene}) \left( \frac{\text{mol pyrene}}{202 \text{ g pyrene}} \right) \left( \frac{6 \text{ mol } F_3O_4}{\text{mol pyrene}} \right) \left( \frac{231.6 \text{ g } F_3O_4}{\text{mol } F_3O_4} \right) = 0.34 \text{ g } F_3O_4
 \end{aligned}$$

$$\begin{aligned}
 &2MnO_2 + H_2O \rightarrow Mn_2O_3 + 2H^+ + 2e^- \\
 &C_{16}H_{10} + 6MnO_2 + 3H_2O \rightarrow 3Mn_2O_3 + 8C_2H_2 \\
 \text{Mass of } MnO_2 &= (0.05 \text{ g pyrene}) \left( \frac{\text{mol pyrene}}{202 \text{ g pyrene}} \right) \left( \frac{6 \text{ mol } MnO_2}{\text{mol pyrene}} \right) \left( \frac{86.9 \text{ g } MnO_2}{\text{mol } MnO_2} \right) = 0.12 \text{ g } MnO_2
 \end{aligned}$$

**Table S6.** Fe(III):Fe(II) ratios of magnetite samples treated under various conditions calculated from XPS Fe 2p peaks.

Sample	Fe(III):Fe(II)	Std Dev
Untreated	7.3	1.69
250 °C for 30 min in N <sub>2</sub>	5.4	1.9
250 °C for 30 min in N <sub>2</sub> with 0.050 g pyrene	7.2	7.3
250 °C for 30 min in air with 100 uL H <sub>2</sub> O	4.9	2.6
250 °C for 30 min in air with 0.050 g pyrene and 100 uL H <sub>2</sub> O	5.0	1.9

## 5. Mössbauer



**Figure S8.** Mössbauer spectra of magnetite blank, magnetite wet and magnetite dry.

**Table S7.** Mössbauer parameters of magnetite samples derived from fitting spectra collected at 140 K.

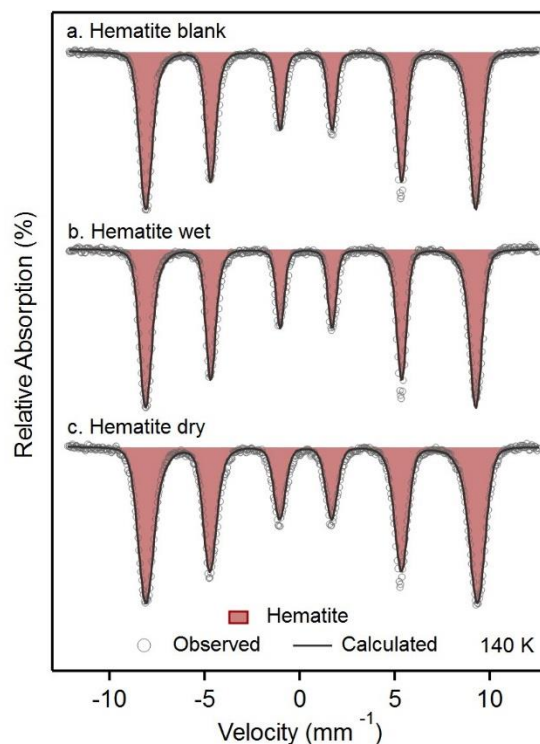
		CS <sup>a</sup> (mm/s)	QS <sup>b</sup> (mm/s)	H <sup>c</sup> (T)	Std(H) (T)	Area (%)
Magnetite blank	Fe <sup>3+</sup>	0.39	-0.021	51.1	1.17	57.5
	Fe <sup>2.5+</sup>	0.79	0.043	47.3	4.30	42.5
Magnetite wet	Fe <sup>3+</sup>	0.39	-0.011	51.2	1.45	58.7
	Fe <sup>2.5+</sup>	0.79	0.016	47.3	4.30	41.3
Magnetite dry	Fe <sup>3+</sup>	0.41	-0.006	51.4	1.49	64.2
	Fe <sup>2.5+</sup>	0.79	-0.016	45.8	8.10	35.8

<sup>a</sup> Center shift

<sup>b</sup> Quadrupole shift

<sup>c</sup> Hyperfine Field

<sup>d</sup> Standards deviation of the Voigt profile for the hyperfine field



**Figure S9.** Mössbauer spectra of hematite blank, hematite wet and hematite dry.

**Table S8.** Mössbauer parameters of magnetite samples derived from fitting spectra collected at 140 K.

	CS <sup>a</sup> (mm/s)	QS <sup>b</sup> (mm/s)	H <sup>c</sup> (T)	Std(H) (T)	Area (%)
Hematite blank	0.47	0.122	53.4	1.95	100
Hematite wet	0.46	0.120	53.5	1.95	100.0
Hematite dry	0.47	0.159	53.5	2.51	100.0

<sup>a</sup> Center shift

<sup>b</sup> Quadrupole shift

<sup>c</sup> Hyperfine Field

<sup>d</sup> Standards deviation of the Voigt profile for the hyperfine field



## 6. By-Product Oxidation States

**Table S9:** Average oxidation state of carbons atoms in byproducts detected from concentrated extracts in mineral limited experiments with magnetite in a dry environment.

<i>Temp</i> (°C)	<i>Compound</i>	<i>Formula</i>	<i>Avg C</i> <i>Ox State</i>
500	Octane, 4,5-diethyl-	C12H26	-2.17
500	Decane, 5,6-dimethyl-	C12H26	-2.17
500	Undecane, 5-methyl-	C12H26	-2.17
500	Cyclohexane, 3-ethyl-5-methyl-1-propyl-	C12H24	-2.00
500	Cyclohexane, (1,2-dimethylbutyl)-	C12H24	-2.00
500	Cyclohexane, undecyl-	C17H34	-2.00
500	Cyclohexane, octyl-	C14H28	-2.00
500	Naphthalene	C10H8	-0.80
300	Anthracene, 9-ethenyl-	C16H12	-0.75
100	Acephenanthrylene, 4,5-dihydro-	C16H12	-0.75
500	Phenanthrene	C14H10	-0.71
500	Pyrene, 1-methyl-	C17H12	-0.71
100	7H-Benzo[c]fluorene	C17H12	-0.71
100	11H-Benzo[b]fluorene	C17H12	-0.71
100	11H-Benzo[a]fluorene	C17H12	-0.71
100	4H-Cyclopenta[def]phenanthrene	C15H10	-0.67
500	Pyrene, 1-phenyl-	C22H14	-0.64
300	Fluoranthene	C16H10	-0.63
	Pyrene	C16H10	-0.63
500	Perylene	C20H12	-0.60
500	Benzo[ghi]perylene	C22H12	-0.55
500	Indeno[1,2,3-cd]pyrene	C22H12	-0.55

**Table S10:** Average oxidation state of carbons atoms in byproducts detected from concentrated extracts in mineral limited experiments with magnetite in a saturated environment.

<i>Temp (°C)</i>	<i>Compound</i>	<i>Formula</i>	<i>Avg C Ox State</i>
300	Heptane, 3,4,5-trimethyl-	C10H22	-2.20
500	Decane, 5,6-dimethyl-	C12H26	-2.17
500	Undecane, 5-methyl-	C12H26	-2.17
300	Octane, 4,5-diethyl-	C12H26	-2.17
500	Cyclohexane, octyl-	C14H28	-2.15
300	Undecane, 4,4-dimethyl-	C13H28	-2.15
500	Cyclohexane, 3-ethyl-5-methyl-1-propyl-	C12H24	-2.00
300	Cyclohexane, (1,2-dimethylbutyl)-	C12H24	-2.00
300	Cyclohexane, (1-methylethyl)-	C14H28	-2.00
300	Isobutyl stearate	C22H44O2	-1.82
500	3-n-Propyl-5-methylhexan-2-one	C10H20O	-1.80
500	Cyclohexaneethanol	C8H16O	-1.75
500	3-Hexanone	C6H12O	-1.67
500	5,8-Tridecadione	C13H24O2	-1.54
300	3-n-Propyl-2,4-pentanedione	C8H14O2	-1.25
500	Biphenyl	C12H10	-0.83
300	Pyrene, 1,3-dimethyl-	C18H14	-0.78
500	1H-Indene, 1-(phenylmethylene)-	C16H12	-0.75
100	Anthracene, 9-ethenyl-	C16H12	-0.75
500	Phenanthrene	C14H10	-0.71
500	Pyrene, 1-methyl-	C17H12	-0.71
100	11H-Benzo[a]fluorene	C17H12	-0.71
100	7H-Benzanthrene	C17H12	-0.71
500	Cyclopenta(cd)pyrene, 3,4-dihydro-	C18H12	-0.67
100	Cyclopenta[def]phenanthrene	C15H10	-0.67
500	Pyrene, 1-phenyl-	C22H14	-0.64
500	Pentacene	C22H14	-0.64
500	5-Methoxy-benzo[c]phenanthrene	C19H14O	-0.63
	Pyrene	C16H10	-0.63
500	Benzophenone	C13H10O	-0.62
500	Benzo[e]pyrene	C20H12	-0.60
500	Indeno[1,2,3-cd]pyrene	C22H12	-0.55
500	Naphtho[2,1-b]furan	C12H8O	-0.50
500	Dibenzofuran	C12H8O	-0.50
300	1-Hydroxypyrene	C16H10O	-0.50
500	1H-Phenalen-1-one	C13H8O	-0.46
500	Naphtho[2,1,8,7-klmn]xanthene	C18H10O	-0.44
500	Cyclopenta(def)phenanthrenone	C15H8O	-0.40