

Table S6. Results of GC–MS analysis of volatiles extracted by mechanical shock crushing from pyrrhotite (Blagodatnoye deposit, Yenisei ridge).

Formula	Name	¹ CAS/(NIST)	² MW	Pyrrhotite 34/105.9	
				³ RT, min	⁴ A, %
Aliphatic hydrocarbons					
Paraffins					
CH4	Methane	74-82-8	16	1.80	0.329
C3H8	n-Propane	74-98-6	44	3.88	0.024
C4H10	n-Butane	106-97-8	58	5.91	0.003
C5H12	n-Pentane	109-66-0	72	7.69	0.137
C6H14	n-Hexane	110-54-3	86	11.42	0.048
C7H16	n-Heptane	142-82-5	100	15.34	0.024
C8H18	3-Methylheptane	589-81-1	114	18.54	0.029
C8H18	n-Octane	111-65-9	114	19.37	0.041
C9H20	n-Nonane	111-84-2	128	23.20	0.047
C10H22	n-Decane	124-18-5	142	26.76	0.024
C11H24	n-Undecane	1120-21-4	156	30.06	0.035
C12H26	n-Dodecane	112-40-3	170	33.62	0.033
C13H28	n-Tridecane	629-50-5	184	36.57	0.018
C14H30	n-Tetradecane	629-59-4	198	41.73	0.020
C15H32	n-Pentadecane	629-62-9	212	49.73	0.028
Halogenated paraffins					
C10H21Cl	1-Chlorodecane	1002-69-3	176	36.41	0.026
Olefins					
C4H8	2-Methyl-1-propene	115-11-7	56	5.53	0.013
C4H8	1-Butene	106-98-9	56	5.73	0.040
C4H8	2-Butene	107-01-7	56	5.93	0.018
C4H8	(E)-2-Butene	624-64-6	56	6.03	0.012
C5H8	(E)-1,3-Pentadiene	2004-70-8	68	7.78	0.005
C5H8	1,3-Pentadiene	504-60-9	68	8.16	0.018
C5H8	(Z)-1,3-Pentadiene	1574-41-0	68	8.63	0.004
C6H12	1-Hexene	592-41-6	84	11.12	0.002
C6H12	2-Hexene	592-43-8	84	11.29	0.001
C6H10	2,3-Dimethyl-1,3-butadiene	513-81-5	82	12.21	0.005
C6H10	3-Hexyne	928-49-4	82	12.46	0.002
C6H10	(E)-2-Methyl-1,3-pentadiene	926-54-5	82	12.76	0.002
C7H14	1-Heptene	592-76-7	98	15.00	0.016
C8H16	(Z)-3-Octene	14850-22-7	112	18.73	0.006
C8H16	(E)-2-Octene	13389-42-9	112	18.97	0.004
C8H16	(Z)-2-Octene	7642-04-8	112	19.03	0.002
C8H16	1-Octene	111-66-0	112	19.15	0.004
C8H16	2-Octene	111-67-1	112	19.25	0.001
C8H16	3-Methyl-2-heptene	3404-75-9	112	19.48	0.001

C ₉ H ₁₈	1-Nonene	124-11-8	126	22.95	0.014
C ₁₀ H ₂₀	1-Decene	872-05-9	140	26.55	0.005
C ₁₁ H ₂₂	1-Undecene	821-95-4	154	29.86	0.016
C ₁₂ H ₂₄	1-Dodecene	112-41-4	168	33.11	0.002
C ₁₃ H ₂₆	1-Tridecene	2437-56-1	182	36.37	0.036
C ₁₄ H ₂₈	1-Tetradecene	1120-36-1	196	41.43	0.048
C ₁₅ H ₃₀	1-Pentadecene	13360-61-7	210	49.28	0.077
C ₁₆ H ₃₂	1-Hexadecene	629-73-2	224	61.86	0.607
Cyclic hydrocarbons					
<i>Cycloalkanes (naphthenes) and cycloalkenes</i>					
C ₅ H ₁₀	Cyclopentane	287-92-3	70	8.28	0.013
C ₆ H ₁₀	3-Methylcyclopentene	1120-62-3	82	11.56	0.004
C ₆ H ₁₀	4-Methylcyclopentene	1759-81-5	82	11.89	0.001
<i>Arenes</i>					
C ₆ H ₆	Benzene	71-43-2	78	11.97	0.009
C ₇ H ₈	Toluene	108-88-3	92	16.32	0.024
C ₇ H ₇ F	(Fluoromethyl)benzene	350-50-5	110	19.92	0.001
C ₈ H ₁₀	Ethylbenzene	100-41-4	106	20.30	0.014
C ₈ H ₁₀	p-Xylene	106-42-3	106	20.57	0.057
C ₈ H ₁₀	o-Xylene	95-47-6	106	20.67	0.004
C ₈ H ₁₀	m-Xylene	108-38-3	106	20.85	0.003
C ₈ H ₈	Styrene	100-42-5	104	21.25	0.004
C ₈ H ₉ F	p-Fluoroethylbenzene	459-47-2	124	22.88	0.029
C ₉ H ₁₂	Propylbenzene	103-65-1	120	24.08	0.020
C ₁₀ H ₁₂	3-Butenylbenzene	768-56-9	132	25.05	0.030
C ₁₀ H ₁₄	Butylbenzene	104-51-8	134	27.81	0.021
C ₁₁ H ₁₆	Pentylbenzene	538-68-1	148	31.17	0.025
C ₁₂ H ₁₈	(2-Methylpentyl)-benzene	39916-61-5	162	31.56	0.020
C ₁₂ H ₁₈	Hexylbenzene	1077-16-3	162	34.37	0.030
C ₁₃ H ₂₀	Heptylbenzene	1078-71-3	176	38.59	0.035
C ₁₄ H ₂₂	1-(1-Ethylpropyl)-4-propylbenzene	54789-16-1	190	43.05	0.032
C ₁₄ H ₂₂	Octylbenzene	2189-60-8	190	44.95	0.029
C ₁₅ H ₂₄	(2-Methyloctyl)-benzene	49826-80-4	204	53.35	0.073
C ₁₅ H ₂₄	Nonylbenzene	1081-77-2	204	54.90	0.070
C ₁₆ H ₂₆	Decylbenzene (1/2)	x	218	69.60	0.069
C ₁₆ H ₂₆	Decylbenzene (2/2)	104-72-3	218	70.79	0.047
<i>PAH (Polycyclic aromatic hydrocarbons)</i>					
C ₁₀ H ₈	Naphthalene	91-20-3	128	31.36	0.004
C ₁₄ H ₁₀	Phenanthrene	85-01-8	178	78.41	0.005
C ₁₄ H ₁₀	Anthracene	120-12-7	178	79.96	0.003
Oxygenated hydrocarbons					
<i>Alcohols</i>					
CH ₄ O	Methanol	67-56-1	32	4.86	0.053

C ₂ H ₆ O	Ethanol	64-17-5	46	6.10	0.120
C ₃ H ₈ O	Isopropyl Alcohol	67-63-0	60	7.81	0.006
C ₄ H ₁₀ O	1-Butanol	71-36-3	74	12.51	0.058
C ₆ H ₁₂ O	(E)-2-Hexen-1-ol	928-95-0	100	19.63	0.032
C ₆ H ₆ O	Phenol	108-95-2	94	24.08	0.029
C ₇ H ₈ O	2-Methylphenol	95-48-7	108	25.43	0.002
C ₆ H ₁₂ O ₂	Tetrahydro-2H-pyran-2-methanol	100-72-1	116	26.70	0.006
C ₇ H ₈ O	3-Methylphenol	108-39-4	108	26.71	0.004
C ₇ H ₈ O	4-Methylphenol	106-44-5	108	27.56	0.006
C ₁₀ H ₂₀ O	(E)-2-Decen-1-ol	18409-18-2	156	34.07	0.034
C ₁₄ H ₃₀ O	3-Tetradecanol	1653-32-3	214	52.41	0.010
<i>Ethers and esters</i>					
C ₅ H ₈ O ₂	Methyl methacrylate	80-62-6	100	13.92	0.035
C ₄ H ₆ O ₂	Butyrolactone	96-48-0	86	20.60	0.005
C ₆ H ₁₀ O ₂	γ-Hexalactone	695-06-7	114	27.00	0.004
C ₇ H ₁₂ O ₂	γ-Heptalactone	105-21-5	128	30.51	0.013
C ₈ H ₁₄ O ₂	γ-Octalactone	104-50-7	142	33.84	0.006
C ₉ H ₁₆ O ₂	γ-Nonalactone	104-61-0	156	35.51	0.015
C ₁₀ H ₁₈ O ₂	γ-Decalactone	706-14-9	170	43.90	0.009
C ₁₁ H ₂₀ O ₂	γ-Undecalactone	104-67-6	184	51.65	0.010
C ₁₂ H ₁₄ O ₄	Diethyl Phthalate	84-66-2	222	52.73	0.004
C ₁₂ H ₂₀ O ₂	γ-6-(Z)-Dodecenolactone	18679-18-0	196	66.72	0.018
C ₁₂ H ₂₂ O ₂	γ-Dodecalactone	2305-05-7	198	68.05	0.011
C ₁₂ H ₂₂ O ₂	10-Methylundecan-5-olide	(370407)	198	73.85	0.019
C ₁₂ H ₂₂ O ₂	δ-Dodecalactone	713-95-1	198	75.12	0.004
C ₁₃ H ₂₄ O ₂	γ-Tridecalactone	x	212	90.96	0.016
C ₁₄ H ₂₆ O ₂	γ-Tetradecalactone	x	226	129.48	0.181
<i>Aldehydes</i>					
C ₂ H ₄ O	Acetaldehyde	75-07-0	44	5.20	0.102
C ₃ H ₄ O	2-Propenal	107-02-8	56	7.09	0.009
C ₃ H ₆ O	n-Propanal	123-38-6	58	7.34	0.027
C ₄ H ₆ O	2-Methyl-2-propenal	78-85-3	70	9.36	0.005
C ₄ H ₈ O	2-Methylpropanal	78-84-2	72	9.43	0.004
C ₄ H ₈ O	n-Butanal	123-72-8	72	10.18	0.008
C ₅ H ₁₀ O	3-Methylbutanal	590-86-3	86	13.24	0.001
C ₅ H ₁₀ O	n-Pentanal	110-62-3	86	14.19	0.015
C ₅ H ₈ O	3-Methyl-2-butenal	107-86-8	84	16.75	0.003
C ₅ H ₄ O ₂	Furfural	98-01-1	96	16.96	0.002
C ₅ H ₄ O ₂	3-Furaldehyde	498-60-2	96	17.77	0.020
C ₆ H ₁₂ O	n-Hexanal	66-25-1	100	18.44	0.047
C ₇ H ₁₄ O	n-Heptanal	111-71-7	114	22.50	0.031
C ₇ H ₆ O	Benzaldehyde	100-52-7	106	23.50	0.053

C ₈ H ₁₆ O	2-Ethylhexanal	123-05-7	128	24.91	0.009
C ₈ H ₁₆ O	n-Octanal	124-13-0	128	26.25	0.031
C ₆ H ₄ O ₃	2,5-Furandicarboxaldehyde	823-82-5	124	27.33	0.013
C ₇ H ₁₂ O	2-Ethyl-4-pentenal	5204-80-8	112	29.18	0.092
C ₉ H ₁₈ O	n-Nonanal	124-19-6	142	29.69	0.047
C ₁₀ H ₂₀ O	n-Decanal	112-31-2	156	32.89	0.056
C ₁₂ H ₂₄ O	2-Methylundecanal	110-41-8	184	38.84	0.004
C ₁₃ H ₂₆ O	n-Tridecanal	10486-19-8	198	47.68	0.105
C ₁₄ H ₂₈ O	n-Tetradecanal	124-25-4	212	60.43	0.062
C ₁₅ H ₃₀ O	13-Methyltetradecanal	75853-51-9	226	80.65	0.107
C ₁₅ H ₃₀ O	n-Pentadecanal	2765-11-9	226	81.61	0.104
C ₁₆ H ₃₂ O	n-Hexadecanal	629-80-1	240	112.92	0.126
<i>Ketones</i>					
C ₃ H ₆ O	2-Propanone	67-64-1	58	7.39	0.018
C ₄ H ₆ O	2-Butenone	78-94-4	70	10.01	0.002
C ₄ H ₆ O ₂	2,3-Butanedione	431-03-8	86	10.26	0.002
C ₄ H ₈ O	2-Butanone	78-93-3	72	10.36	0.005
C ₅ H ₁₀ O	2-Pentanone	107-87-9	86	13.99	0.015
C ₅ H ₈ O	Cyclopentanone	120-92-3	84	16.44	0.021
C ₆ H ₁₂ O	2-Hexanone	591-78-6	100	18.22	0.013
C ₇ H ₁₄ O	2-Heptanone	110-43-0	114	22.23	0.030
C ₈ H ₁₆ O	2-Octanone	111-13-7	128	26.96	0.016
C ₉ H ₁₈ O	2-Nonanone	821-55-6	142	29.39	0.023
C ₁₀ H ₂₀ O	2-Decanone	693-54-9	156	32.57	0.015
C ₈ H ₄ O ₃	1,3-Isobenzofurandione	85-44-9	148	32.17	0.181
C ₁₁ H ₂₂ O	2-Undecanone	53452-70-3	170	35.92	0.017
C ₁₂ H ₂₄ O	2-Dodecanone	6175-49-1	184	40.73	0.017
C ₁₃ H ₂₆ O	3-Tridecanone	1534-26-5	198	46.60	0.073
C ₁₃ H ₂₆ O	2-Tridecanone	593-08-8	198	48.21	0.048
C ₁₄ H ₂₈ O	2-Tetradecanone	2345-27-9	212	58.61	0.045
C ₁₃ H ₁₆ O ₂	(1-Hydroxycyclohexyl) phenyl methanone	947-19-3	204	72.57	0.016
C ₁₅ H ₃₀ O	3-Methyl-2-tetradecanone	x	226	77.56	0.157
C ₁₅ H ₃₀ O	2-Pentadecanone	2345-28-0	226	78.70	0.089
C ₁₆ H ₃₂ O	2-Hexadecanone	18787-63-8	240	108.41	0.108
<i>Carboxylic acids</i>					
CH ₂ O ₂	Formic acid	64-18-6	46	6.11	0.158
C ₂ H ₄ O ₂	Acetic acid	64-19-7	60	10.91	0.288
C ₃ H ₆ O ₂	n-Propanoic acid	79-09-4	74	14.66	0.012
C ₄ H ₈ O ₂	n-Butanoic acid	107-92-6	88	18.29	0.191
C ₅ H ₁₀ O ₂	3-Methylbutanoic acid	503-74-2	102	21.23	0.024
C ₅ H ₁₀ O ₂	n-Pentanoic acid	109-52-4	102	22.18	0.072
C ₆ H ₁₂ O ₂	n-Hexanoic acid	142-62-1	116	25.70	0.187
C ₇ H ₁₄ O ₂	3-Methylhexanoic acid	3780-58-3	130	28.09	0.158

C ₇ H ₁₄ O ₂	n-Heptanoic acid	111-14-8	130	29.04	0.086
C ₈ H ₁₆ O ₂	3-Methylheptanoic acid	59614-85-6	144	32.12	0.145
C ₈ H ₁₆ O ₂	n-Octanoic acid	124-07-2	144	33.02	0.198
C ₉ H ₁₈ O ₂	n-Nonanoic acid	112-05-0	158	35.24	0.118
C ₁₀ H ₂₀ O ₂	4-Methylnonanoic acid	45019-28-1	172	37.82	0.247
C ₁₀ H ₂₀ O ₂	n-Decanoic acid	334-48-5	172	39.62	1.962
C ₈ H ₁₄ O ₃	3-Methoxycyclohexanecarboxylic acid	(453574)	158	41.97	0.017
C ₁₁ H ₂₂ O ₂	3-Methyldecanoic acid	60308-82-9	186	45.00	0.031
C ₁₁ H ₂₂ O ₂	n-Undecanoic acid	112-37-8	186	46.55	0.050
C ₁₂ H ₂₄ O ₂	3-Methylundecanoic acid	65781-38-6	200	56.13	0.088
C ₁₂ H ₂₄ O ₂	n-Dodecanoic acid	143-07-7	200	57.10	0.383
C ₁₃ H ₂₆ O ₂	n-Tridecanoic acid	638-53-9	214	74.63	0.106
C ₁₄ H ₂₈ O ₂	n-Tetradecanoic acid	544-63-8	228	101.88	1.191
Heterocyclic compounds					
<i>Dioxanes</i>					
C ₄ H ₈ O ₂	1,4-Dioxane	123-91-1	88	13.22	0.001
<i>Furans</i>					
C ₅ H ₆ O	2-Methylfuran	534-22-5	82	9.83	0.018
C ₅ H ₆ O	3-Methylfuran	930-27-8	82	10.11	<0.001
C ₆ H ₈ O	2-Ethylfuran	3208-16-0	96	13.44	0.001
C ₆ H ₆ O	2-Vinylfuran	1487-18-9	94	14.22	0.002
C ₈ H ₁₂ O	2-Butylfuran	4466-24-4	124	21.52	0.001
C ₉ H ₁₄ O	2-Pentylfuran	3777-69-3	138	25.30	0.002
Nitrogenated compounds					
N ₂	Nitrogen	7727-37-9	28	1.78	1.271
H ₃ N	Ammonia	7664-41-7	17	2.95	0.054
C ₂ H ₃ N	Acetonitrile	75-05-8	41	6.43	0.179
C ₃ H ₅ N	Propargylamine	2450-71-7	55	9.19	0.003
C ₃ H ₈ N ₂	1,2-Dimethyldiaziridine	6794-95-2	72	10.77	0.018
C ₄ H ₅ N	Pyrrole	109-97-7	67	14.12	0.010
C ₂ H ₅ NO	Acetamide	60-35-5	59	16.10	0.029
C ₅ H ₅ N	Pyridine	110-86-1	79	15.22	0.008
C ₃ H ₅ NO ₂	2-Oxo-propionamide	x	87	17.15	0.003
C ₆ H ₉ N	2,3-Dimethyl-1H-pyrrole	600-28-2	95	17.99	0.002
C ₆ H ₇ N	2-Methylpyridine	109-06-8	93	18.45	0.003
C ₆ H ₇ N	3-Methylpyridine	108-99-6	93	20.17	0.002
C ₆ H ₇ N	4-Methylpyridine	108-89-4	93	20.37	0.001
C ₄ H ₉ NO	2-Methylpropanamide	563-83-7	87	23.41	0.006
C ₅ H ₁₁ NO	Pentanamide	626-97-1	101	27.19	0.003
C ₆ H ₁₃ NO	Hexanamide	628-02-4	115	30.63	0.013
C ₇ H ₁₅ NO	Heptamide	628-62-6	129	33.82	0.003
C ₅ H ₇ NO ₂	2,6-Piperidinedione	1121-89-7	113	30.78	0.028

C ₉ H ₁₉ NO	Nonanamide	1120-07-6	157	43.50	0.006
C ₁₀ H ₂₁ NO	Decanamide	2319-29-1	171	50.96	0.018
C ₁₁ H ₂₁ NO ₃	n-Propyl ester hexanoyl glycine	(453014)	215	71.52	0.006
C ₁₂ H ₂₅ NO	Dodecanamide	1120-16-7	199	89.16	0.042
Sulfonated compounds					
H ₂ S	Hydrogen sulfide	7783-06-4	34	2.73	0.359
COS	Carbonyl sulfide	463-58-1	60	3.30	0.004
O ₂ S	Sulfur dioxide	7446-09-5	64	4.58	3.284
CH ₄ S	Methanethiol	74-93-1	48	5.35	0.069
CS ₂	Carbon disulfide	75-15-0	76	7.68	0.087
C ₄ H ₄ S	Thiophene	110-02-1	84	11.76	0.004
C ₂ H ₆ S ₂	Dimethyl disulfide	624-92-0	94	14.74	0.006
C ₅ H ₆ S	2-Methylthiophene	554-14-3	98	15.84	0.008
C ₅ H ₆ S	3-Methylthiophene	616-44-4	98	16.17	0.011
C ₆ H ₈ S	2-Ethylthiophene	872-55-9	112	20.87	0.002
C ₁₀ H ₁₆ S	2-Hexylthiophene	18794-77-9	168	34.19	0.014
Inorganic compounds					
<i>Oxides</i>					
CO ₂	Carbon dioxide	124-38-9	44	1.88	10.034
H ₂ O	Water	7732-18-5	18	3.18	73.454
<i>Noble gases</i>					
Ar	Argon	7440-37-1	40	1.67	0.008

Note: ¹CAS/(NIST) – unique numerical identifier of chemical compounds included in the register Chemical Abstracts Service (<https://www.cas.org>) or NIST number (a unique number given to each spectrum in the NIST archive); ²MW – nominal mass; ³RT – retention time; ⁴A – normalized area (the area ratio of the individual gas mixture components to the sum of the areas of all the components in the chromatogram).