

Table S10. Results of GC–MS analysis of volatiles extracted by mechanical shock crushing from pyrite (Blagodatnoye deposit, Yenisei ridge).

Formula	Name	¹ CAS	² MW	Pyrite 100/216.5	
				³ RT, min	⁴ A, %
Aliphatic hydrocarbons					
Paraffins					
CH4	Methane	74-82-8	16	1.72	1.207
C2H6	Ethane	74-84-0	30	2.70	0.001
C6H14	n-Hexane	110-54-3	86	12.02	0.011
C7H16	n-Heptane	142-82-5	100	16.05	0.005
C8H18	n-Octane	111-65-9	114	20.15	0.008
C9H20	n-Nonane	111-84-2	128	24.03	0.008
C10H22	n-Decane	124-18-5	142	27.61	0.006
C11H24	n-Undecane	1120-21-4	156	30.94	0.007
C12H26	n-Dodecane	112-40-3	170	34.05	0.004
C13H28	n-Tridecane	629-50-5	184	38.03	0.006
C14H30	n-Tetradecane	629-59-4	198	44.10	0.007
C15H32	n-Pentadecane	629-62-9	212	53.57	0.014
Halogenated paraffins					
C4H9Cl	1-Chlorobutane	109-69-3	92	12.64	0.003
Olefins					
C2H2	Acetylene	74-86-2	26	2.22	0.002
C2H4	Ethylene	74-85-1	28	2.43	0.006
C4H8	2-Methyl-1-propene	115-11-7	56	5.93	0.017
C4H8	2-Butene	107-01-7	56	6.15	0.004
C5H10	2-Methyl-2-butene	513-35-9	70	8.29	0.004
C5H8	1,3-Pentadiene	1574-41-0	68	8.54	0.007
C5H8	(E)-1,3-Pentadiene	2004-70-8	68	8.64	0.001
C5H8	(Z)-1,3-Pentadiene	1574-41-0	68	9.04	<0.001
C6H12	1-Hexene	592-41-6	84	11.67	0.004
C7H14	1-Heptene	592-76-7	98	15.70	0.003
C8H16	(Z)-3-Octene	14850-22-7	112	19.55	0.001
C8H16	(E)-2-Octene	13389-42-9	112	19.72	0.001
C8H16	(Z)-2-Octene	7642-04-8	112	19.83	0.002
C8H16	1-Octene	111-66-0	112	19.95	0.002
C9H18	1-Nonene	124-11-8	126	23.75	0.001
C10H20	1-Decene	872-05-9	140	27.39	0.002
C11H22	1-Undecene	821-95-4	154	30.74	0.002
C12H24	1-Dodecene	112-41-4	168	33.89	0.001
C13H26	1-Tridecene	2437-56-1	182	37.79	0.004
C14H28	1-Tetradecene	1120-36-1	196	43.68	0.004
C15H30	1-Pentadecene	13360-61-7	210	52.97	0.025
Cyclic hydrocarbons					
Cycloalkanes (naphthenes) and cycloalkenes					
C5H10	Cyclopentane	287-92-3	70	8.66	0.003

C ₆ H ₁₂	Cyclohexane	110-82-7	84	15.74	0.002
<i>Arenes</i>					
C ₆ H ₆	Benzene	71-43-2	78	12.59	0.017
C ₇ H ₈	Toluene)	108-88-3	92	17.04	0.003
C ₇ H ₇ F	(Fluoromethyl)benzene	350-50-5	110	20.70	<0.001
C ₈ H ₁₀	Ethylbenzene	100-41-4	106	21.08	0.002
C ₈ H ₁₀	p-Xylene	106-42-3	106	21.35	0.004
C ₈ H ₁₀	o-Xylene	95-47-6	106	21.53	<0.001
C ₈ H ₁₀	m-Xylene	108-38-3	106	21.60	<0.001
C ₈ H ₈	Styrene	100-42-5	104	22.00	0.001
C ₉ H ₁₂	Propylbenzene	103-65-1	120	24.90	0.005
C ₁₀ H ₁₄	Butylbenzene	104-51-8	134	28.66	0.010
C ₁₁ H ₁₆	Pentylbenzene	538-68-1	148	32.06	0.011
C ₁₂ H ₁₈	Hexylbenzene	1077-16-3	162	35.52	0.003
C ₁₃ H ₂₀	Heptylbenzene	1078-71-3	176	40.40	0.003
C ₁₄ H ₂₂	Octylbenzene	2189-60-8	190	59.58	0.002
Oxygenated hydrocarbons					
<i>Alcohols</i>					
CH ₄ O	Methanol	67-56-1	32	4.48	0.088
C ₂ H ₆ O	Ethanol	64-17-5	46	6.35	0.003
C ₃ H ₈ O	Isopropyl Alcohol	67-63-0	60	8.04	<0.001
C ₃ H ₈ O	1-Propanol	71-23-8	60	9.11	0.002
C ₄ H ₁₀ O	1-Butanol	71-36-3	74	12.91	0.018
C ₆ H ₆ O	Phenol	108-95-2	94	24.73	0.003
C ₇ H ₈ O	3-Methylphenol	108-39-4	108	27.44	<0.001
C ₇ H ₈ O	4-Methylphenol	106-44-5	108	28.28	0.001
<i>Ethers and esters</i>					
C ₅ H ₈ O ₂	Methyl methacrylate	80-62-6	100	14.45	<0.001
C ₇ H ₁₂ O ₂	γ-Heptalactone	105-21-5	128	31.07	<0.001
C ₈ H ₁₄ O ₂	γ-Octalactone	104-50-7	142	34.54	0.004
C ₉ H ₁₆ O ₂	γ-Nonalactone	104-61-0	156	39.05	0.002
C ₁₀ H ₁₈ O ₂	γ-Decalactone	706-14-9	170	45.86	0.004
C ₁₂ H ₁₆ O ₂	Pentyl ester benzoic acid	2049-96-9	192	49.48	0.014
C ₁₃ H ₁₈ O ₂	Hexyl ester benzoic acid	6789-88-4	206	59.18	0.007
C ₁₂ H ₁₄ O ₄	Diethyl phthalate	84-66-2	222	69.49	0.038
C ₁₂ H ₂₂ O ₂	γ-Dodecalactone	2305-05-7	198	73.60	0.011
C ₁₄ H ₁₈ O ₄	Dipropyl ester 1,2-benzenedicarboxylic acid	131-16-8	250	111.32	0.080
<i>Aldehydes</i>					
C ₂ H ₄ O	Acetaldehyde	75-07-0	44	5.26	0.030
C ₃ H ₄ O	2-Propenal	107-02-8	56	7.24	0.007
C ₃ H ₆ O	n-Propanal	123-38-6	58	7.46	0.020
C ₄ H ₆ O	2-Methyl-2-propenal	78-85-3	70	9.73	0.003

C ₄ H ₈ O	2-Methylpropanal	78-84-2	72	9.74	0.001
C ₄ H ₈ O	n-Butanal	123-72-8	72	10.54	0.003
C ₅ H ₁₀ O	3-Methylbutanal	590-86-3	86	13.67	0.004
C ₅ H ₁₀ O	n-Pentanal	110-62-3	86	14.65	0.001
C ₅ H ₄ O ₂	Furfural	98-01-1	96	17.45	<0.001
C ₆ H ₁₀ O	2-Methyl-2-pentenal	623-36-9	98	18.10	<0.001
C ₅ H ₄ O ₂	3-Furaldehyde	498-60-2	96	18.32	0.003
C ₆ H ₁₂ O	n-Hexanal	66-25-1	100	19.00	0.008
C ₇ H ₁₄ O	n-Heptanal	111-71-7	114	23.13	0.004
C ₆ H ₆ O ₂	5-Methyl-2-furancarboxaldehyde	620-02-0	110	23.38	0.001
C ₆ H ₄ O ₃	2,5-Furandicarboxaldehyde	823-82-5	124	27.74	0.002
C ₇ H ₆ O	Benzaldehyde	100-52-7	106	24.10	0.011
C ₈ H ₁₆ O	2-Ethylhexanal	123-05-7	128	25.61	0.038
C ₈ H ₁₆ O	n-Octanal	124-13-0	128	26.94	0.010
C ₉ H ₁₈ O	n-Nonanal	124-19-6	142	30.44	0.013
C ₁₀ H ₂₀ O	n-Decanal	112-31-2	156	33.67	0.018
C ₁₁ H ₂₂ O	n-Undecanal	112-44-7	170	37.60	0.006
C ₁₂ H ₂₄ O	n-Dodecanal	112-54-9	184	43.45	0.007
C ₁₁ H ₁₄ O	Benzenepentanal	36884-28-3	162	45.60	0.002
C ₁₄ H ₂₈ O	n-Tetradecanal	124-25-4	212	67.13	0.016
C ₁₅ H ₃₀ O	n-Pentadecanal	2765-11-9	226	90.84	0.020
<i>Ketones</i>					
C ₃ H ₆ O	2-Propanone	67-64-1	58	7.63	0.015
C ₄ H ₆ O ₂	2,3-Butanedione	431-03-8	86	10.62	0.001
C ₄ H ₈ O	2-Butanone	78-93-3	72	10.69	0.001
C ₅ H ₁₀ O	2-Pentanone	107-87-9	86	14.45	0.002
C ₆ H ₁₂ O	2-Hexanone	591-78-6	100	18.73	0.001
C ₇ H ₁₄ O	2-Heptanone	110-43-0	114	22.83	0.003
C ₈ H ₁₆ O	2-Octanone	111-13-7	128	26.64	0.002
C ₉ H ₁₈ O	2-Nonanone	821-55-6	142	30.13	0.001
C ₁₀ H ₂₀ O	2-Decanone	693-54-9	156	33.34	0.002
C ₈ H ₄ O ₃	1,3-Isobenzofurandione	85-44-9	148	35.94	0.022
C ₁₁ H ₂₂ O	2-Undecanone	53452-70-3	170	37.09	0.006
C ₁₂ H ₂₄ O	2-Dodecanone	6175-49-1	184	42.68	0.003
C ₁₃ H ₂₆ O	2-Tridecanone	593-08-8	198	51.37	0.010
C ₁₄ H ₂₈ O	2-Tetradecanone	2345-27-9	212	64.96	0.010
C ₁₅ H ₃₀ O	2-Pentadecanone	2345-28-0	226	87.03	0.030
<i>Carboxylic acids</i>					
C ₂ H ₄ O ₂	Acetic acid	64-19-7	60	11.36	0.052
C ₃ H ₆ O ₂	n-Propanoic acid	79-09-4	74	15.39	0.001
C ₄ H ₈ O ₂	n-Butanoic acid	107-92-6	88	19.03	0.022
C ₅ H ₁₀ O ₂	3-Methylbutanoic acid	503-74-2	102	22.07	0.002
C ₅ H ₁₀ O ₂	n-Pentanoic acid	109-52-4	102	23.06	0.006

C ₆ H ₁₂ O ₂	n-Hexanoic acid	142-62-1	116	26.49	0.045
C ₇ H ₁₄ O ₂	n-Heptanoic acid	111-14-8	130	29.98	0.009
C ₈ H ₁₆ O ₂	n-Octanoic acid	124-07-2	144	32.89	0.178
C ₉ H ₁₈ O ₂	n-Nonanoic acid	112-05-0	158	36.60	0.011
C ₁₀ H ₂₀ O ₂	n-Decanoic acid	334-48-5	172	41.65	0.094
C ₁₂ H ₂₄ O ₂	n-Dodecanoic acid	143-07-7	200	62.06	0.204
C ₁₄ H ₂₈ O ₂	n-Tetradecanoic acid	544-63-8	228	118.88	0.043
Heterocyclic compounds					
<i>Dioxanes</i>					
C ₄ H ₈ O ₂	1,4-Dioxane	123-91-1	88	13.69	0.001
<i>Furans</i>					
C ₅ H ₆ O	2-Methylfuran	534-22-5	82	10.31	0.001
C ₅ H ₆ O	3-Methylfuran	930-27-8	82	10.57	<0.001
C ₆ H ₈ O	2-Ethylfuran	3208-16-0	96	14.14	<0.001
C ₉ H ₁₄ O	2-Pentylfuran	3777-69-3	138	26.10	0.001
Nitrogenated compounds					
N ₂	Nitrogen	7727-37-9	28	1.62	0.608
H ₃ N	Ammonia	7664-41-7	17	2.86	0.025
C ₂ H ₃ N	Acetonitrile	75-05-8	41	6.88	0.003
C ₃ H ₅ N	Propargylamine	2450-71-7	55	9.43	<0.001
C ₄ H ₅ N	Pyrrole	109-97-7	67	14.62	0.001
C ₅ H ₅ N	Pyridine	110-86-1	79	15.52	0.001
C ₃ H ₅ NO ₂	2-Oxo-propionamide	x	87	17.44	0.004
C ₆ H ₉ N	2,3-Dimethyl-1H-pyrrole	600-28-2	95	18.45	<0.001
C ₆ H ₇ N	2-Methylpyridine	109-06-8	93	18.83	<0.001
C ₆ H ₇ N	3-Methylpyridine	108-99-6	93	20.55	<0.001
C ₆ H ₇ N	4-Methylpyridine	108-89-4	93	20.67	<0.001
C ₈ H ₁₉ N	3-Octanamine	24552-04-3	129	25.81	0.001
C ₄ H ₅ NO ₂	Succinimide	123-56-8	99	28.86	0.003
C ₆ H ₁₃ NO	Hexanamide	628-02-4	115	38.70	0.005
C ₉ H ₁₉ NO	Nonanamide	x	157	55.42	0.004
C ₁₁ H ₂₃ NO	Undecanamide	x	185	97.62	0.009
Sulfonated compounds					
H ₂ S	Hydrogen sulfide	7783-06-4	34	2.86	0.022
COS	Carbonyl sulfide	463-58-1	60	3.51	0.004
O ₂ S	Sulfur dioxide	7446-09-5	64	5.06	0.576
CH ₄ S	Methanethiol	74-93-1	48	5.06	0.144
CS ₂	Carbon disulfide	75-15-0	76	7.84	0.008
C ₂ H ₆ S ₂	Dimethyl disulfide	624-92-0	94	15.35	<0.001
C ₅ H ₆ S	2-Methylthiophene	554-14-3	98	16.54	0.001
C ₅ H ₆ S	3-Methylthiophene	616-44-4	98	16.89	0.018
Inorganic compounds					
<i>Oxides</i>					
CO ₂	Carbon dioxide	124-38-9	44	1.88	1.533
H ₂ O	Water	7732-18-5	18	3.21	94.294
<i>Noble gases</i>					

Ar	Argon	7440-37-1	40	1.60	0.009
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Note: ¹CAS – unique numerical identifier of chemical compounds included in the register Chemical Abstracts Service (<https://www.cas.org>); 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).