

Table S4. Results of GC–MS analysis of volatiles extracted by mechanical shock crushing from arsenopyrite (Blagodatnoye deposit, Yenisei ridge).

Formula	Name	¹ CAS/(NIST)	² MW	Arsenopyrite BKS-10	
				³ RT, min	⁴ A, %
Aliphatic hydrocarbons					
Paraffins					
CH4	Methane	74-82-8	16	1.73	3.503
C3H8	n-Propane	74-98-6	44	4.30	0.003
C4H10	n-Butane	106-97-8	58	5.88	0.003
C5H12	n-Pentane	109-66-0	72	7.73	0.006
C6H14	n-Hexane	110-54-3	86	11.21	0.066
C7H16	n-Heptane	142-82-5	100	15.04	0.003
C8H18	n-Octane	111-65-9	114	18.97	0.006
C9H20	n-Nonane	111-84-2	128	22.75	0.008
C10H22	n-Decane	124-18-5	142	26.24	0.004
C11H24	n-Undecane	1120-21-4	156	29.51	0.003
C12H26	n-Dodecane	112-40-3	170	32.52	0.002
C13H28	n-Tridecane	629-50-5	184	35.69	0.008
C14H30	n-Tetradecane	629-59-4	198	40.32	0.011
C15H32	n-Pentadecane	629-62-9	212	47.38	0.013
Olefins					
C4H8	2-Methyl-1-propene	115-11-7	56	5.58	0.001
C4H8	1-Butene	106-98-9	56	5.71	0.001
C4H8	2-Butene	107-01-7	56	5.76	0.001
C5H8	(E)-1,3-Pentadiene	2004-70-8	68	7.98	<0.001
C5H8	1,3-Pentadiene	504-60-9	68	8.09	<0.001
C5H8	(Z)-1,3-Pentadiene	1574-41-0	68	8.28	<0.001
C6H12	1-Hexene	592-41-6	84	10.96	0.052
C6H12	2-Hexene	592-43-8	84	11.12	0.017
C6H12	3-Hexene	592-47-2	84	11.29	0.004
C6H10	2,3-Dimethyl-1,3-butadiene	513-81-5	82	12.06	0.001
C6H10	3-Hexyne	928-49-4	82	12.32	<0.001
C6H10	1(E)-2-Methyl-3-pentadiene	926-54-5	82	12.61	<0.001
C7H14	1-Heptene	592-76-7	98	14.74	0.002
C8H16	1-Octene	111-66-0	112	18.70	0.001
C9H18	1-Nonene	124-11-8	126	22.50	0.002
C10H20	1-Decene	872-05-9	140	26.06	0.001
C13H26	1-Tridecene	2437-56-1	182	35.55	0.005
C14H28	1-Tetradecene	1120-36-1	196	40.05	0.007
C15H30	1-Pentadecene	13360-61-7	210	47.01	0.014
Cyclic hydrocarbons					
Cycloalkanes (naphthenes) and cycloalkenes					
C6H10	3-Methylcyclopentene	1120-62-3	82	11.44	<0.001

C ₆ H ₁₀	4-Methylcyclopentene	1759-81-5	82	11.76	<0.001
C ₆ H ₁₂	Cyclohexane	110-82-7	84	12.87	0.001
<i>Arenes</i>					
C ₆ H ₆	Benzene	71-43-2	78	11.92	0.070
C ₇ H ₈	Toluene	108-88-3	92	16.19	0.005
C ₇ H ₇ F	(Fluoromethyl)benzene	350-50-5	110	19.63	<0.001
C ₈ H ₁₀	Ethylbenzene	100-41-4	106	20.08	0.003
C ₈ H ₁₀	p-Xylene	106-42-3	106	20.37	0.011
C ₈ H ₁₀	o-Xylene	95-47-6	106	20.58	0.002
C ₈ H ₁₀	m-Xylene	108-38-3	106	20.65	0.002
C ₈ H ₈	Styrene	100-42-5	104	21.07	0.001
C ₈ H ₉ F	p-Fluoroethylbenzene	459-47-2	124	22.81	<0.001
C ₉ H ₁₂	Propylbenzene	103-65-1	120	23.80	0.005
C ₁₀ H ₁₄	Butylbenzene	104-51-8	134	27.46	0.005
C ₁₁ H ₁₆	Pentylbenzene	538-68-1	148	30.76	0.006
C ₁₂ H ₁₈	Hexylbenzene	1077-16-3	162	33.89	0.004
C ₁₃ H ₂₀	Heptylbenzene	1078-71-3	176	37.77	0.006
C ₁₄ H ₂₂	Octylbenzene	2189-60-8	190	43.55	0.007
C ₁₅ H ₂₄	Nonylbenzene	1081-77-2	204	52.52	0.006
C ₁₆ H ₂₆	Decylbenzene	104-72-3	218	66.58	0.008
<i>PAH (Polycyclic aromatic hydrocarbons)</i>					
C ₁₀ H ₈	Naphthalene	91-20-3	128	31.16	0.001
C ₁₄ H ₁₀	Phenanthrene	85-01-8	178	78.04	0.001
Oxygenated hydrocarbons					
<i>Alcohols</i>					
CH ₄ O	Methanol	67-56-1	32	4.48	0.226
C ₂ H ₆ O	Ethanol	64-17-5	46	6.31	0.038
C ₄ H ₁₀ O	1-Butanol	71-36-3	74	12.57	0.004
C ₆ H ₆ O	Phenol	108-95-2	94	24.01	0.002
<i>Ethers and esters</i>					
C ₅ H ₈ O ₂	Methyl methacrylate	80-62-6	100	13.79	0.001
C ₄ H ₆ O ₂	Butyrolactone	96-48-0	86	20.86	0.001
C ₆ H ₁₀ O ₂	γ-Hexalactone	695-06-7	114	26.88	0.001
C ₇ H ₁₂ O ₂	γ-Heptalactone	105-21-5	128	30.32	0.001
C ₈ H ₁₄ O ₂	γ-Octalactone	104-50-7	142	33.57	0.001
C ₉ H ₁₆ O ₂	γ-Nonalactone	104-61-0	156	37.39	0.001
C ₁₀ H ₁₈ O ₂	γ-Decalactone	706-14-9	170	42.97	0.002
C ₁₁ H ₂₀ O ₂	γ-Undecalatone	104-67-6	184	51.56	0.001
C ₁₂ H ₁₄ O ₄	Diethyl Phthalate	84-66-2	222	62.22	0.013
C ₁₂ H ₂₂ O ₂	γ-Dodecalactone	2305-05-7	198	65.02	0.003
C ₁₆ H ₂₂ O ₄	Di-sec-butyl phthalate	(373654)	278	79.05	1.725
C ₁₃ H ₂₄ O ₂	γ-Tridecalactone	x	212	86.11	0.002
C ₁₄ H ₂₆ O ₂	γ-Tetradecalactone	x	226	119.89	0.012
C ₁₆ H ₂₂ O ₄	Dibutyl phthalate	84-74-2	278	124.69	0.008
C ₁₇ H ₃₀ O ₄	2-Heptyl isohexyl ester fumaric acid	(348625)	298	130.35	0.006

<i>Aldehydes</i>					
C ₂ H ₄ O	Acetaldehyde	75-07-0	44	4.91	0.028
C ₃ H ₄ O	2-Propenal	107-02-8	56	7.11	0.003
C ₃ H ₆ O	n-Propanal	123-38-6	58	7.31	0.002
C ₄ H ₆ O	2-Methyl-2-propenal	78-85-3	70	9.38	<0.001
C ₄ H ₈ O	2-Methylpropanal	78-84-2	72	9.39	0.001
C ₄ H ₈ O	n-Butanal	123-72-8	72	10.16	0.004
C ₅ H ₁₀ O	3-Methylbutanal	590-86-3	86	13.11	0.002
C ₅ H ₁₀ O	n-Pentanal	110-62-3	86	14.07	0.004
C ₅ H ₄ O ₂	Furfural	98-01-1	96	17.00	<0.001
C ₅ H ₄ O ₂	3-Furaldehyde	498-60-2	96	17.90	0.003
C ₆ H ₁₂ O	n-Hexanal	66-25-1	100	18.22	0.011
C ₇ H ₁₄ O	n-Heptanal	111-71-7	114	22.21	0.004
C ₇ H ₆ O	Benzaldehyde	100-52-7	106	23.41	0.005
C ₈ H ₁₆ O	2-Ethylhexanal	123-05-7	128	24.56	0.004
C ₈ H ₁₆ O	n-Octanal	124-13-0	128	25.90	0.006
C ₆ H ₄ O ₃	2,5-Furandicarboxaldehyde	823-82-5	124	27.33	0.002
C ₉ H ₁₈ O	n-Nonanal	124-19-6	142	29.29	0.012
C ₁₀ H ₂₀ O	n-Decanal	112-31-2	156	33.42	0.013
C ₈ H ₆ O ₃	Piperonal	120-57-0	150	37.19	0.976
C ₁₄ H ₂₈ O	n-Tetradecanal	124-25-4	212	58.42	0.017
C ₁₅ H ₃₀ O	n-Pentadecanal	2765-11-9	226	76.01	0.040
C ₁₆ H ₃₂ O	n-Hexadecanal	629-80-1	240	103.92	0.032
<i>Ketones</i>					
C ₃ H ₆ O	2-Propanone	67-64-1	58	7.51	0.026
C ₄ H ₆ O ₂	2,3-Butanedione	431-03-8	86	10.24	0.003
C ₄ H ₈ O	2-Butanone	78-93-3	72	10.36	0.006
C ₅ H ₁₀ O	2-Pentanone	107-87-9	86	13.89	0.002
C ₅ H ₈ O	Cyclopentanone	120-92-3	84	16.69	<0.001
C ₆ H ₁₂ O	2-Hexanone	591-78-6	100	18.02	0.003
C ₇ H ₁₄ O	2-Heptanone	110-43-0	114	21.95	0.003
C ₈ H ₁₆ O	3-Octanone	106-68-3	128	24.81	0.002
C ₈ H ₁₆ O	2-Octanone	111-13-7	128	25.60	0.006
C ₉ H ₁₈ O	2-Nonanone	821-55-6	142	28.99	0.001
C ₁₀ H ₂₀ O	2-Decanone	693-54-9	156	32.14	0.003
C ₈ H ₄ O ₃	1,3-Isobenzofurandione	85-44-9	148	35.14	0.009
C ₁₁ H ₂₂ O	2-Undecanone	53452-70-3	170	35.24	0.004
C ₁₂ H ₂₄ O	2-Dodecanone	6175-49-1	184	39.65	0.001
C ₁₃ H ₂₆ O	2-Tridecanone	593-08-8	198	46.36	0.010
C ₁₄ H ₂₈ O	2-Tetradecanone	2345-27-9	212	56.29	0.011
C ₁₅ H ₃₀ O	2-Pentadecanone	2345-28-0	226	73.32	0.027
C ₁₆ H ₃₂ O	2-Hexadecanone	18787-63-8	240	99.47	0.010
<i>Carboxylic acids</i>					
CH ₂ O ₂	Formic acid	64-18-6	46	6.33	0.006

C ₂ H ₄ O ₂	Acetic acid	64-19-7	60	10.94	0.053
C ₃ H ₆ O ₂	n-Propanoic acid	79-09-4	74	14.69	0.001
C ₄ H ₈ O ₂	n-Butanoic acid	107-92-6	88	18.18	0.036
C ₅ H ₁₀ O ₂	3-Methylbutanoic acid	503-74-2	102	21.05	0.003
C ₅ H ₁₀ O ₂	n-Pentanoic acid	109-52-4	102	22.06	0.013
C ₆ H ₁₂ O ₂	n-Hexanoic acid	142-62-1	116	25.48	0.043
C ₇ H ₁₄ O ₂	n-Heptanoic acid	111-14-8	130	28.79	0.010
C ₈ H ₁₆ O ₂	n-Octanoic acid	124-07-2	144	31.79	0.028
C ₉ H ₁₈ O ₂	n-Nonanoic acid	112-05-0	158	34.77	0.029
C ₁₀ H ₂₀ O ₂	n-Decanoic acid	334-48-5	172	38.85	0.021
C ₁₁ H ₂₂ O ₂	n-Undecanoic acid	112-37-8	186	45.10	0.004
C ₁₂ H ₂₄ O ₂	n-Dodecanoic acid	143-07-7	200	54.89	0.021
C ₁₄ H ₂₈ O ₂	n-Tetradecanoic acid	544-63-8	228	94.86	0.030
Heterocyclic compounds					
<i>Dioxanes</i>					
C ₄ H ₈ O ₂	1,4-Dioxane	123-91-1	88	13.19	<0.001
<i>Furans</i>					
C ₅ H ₆ O	2-Methylfuran	534-22-5	82	9.81	<0.001
C ₅ H ₆ O	3-Methylfuran	930-27-8	82	9.86	<0.001
C ₆ H ₈ O	2,5-Dimethylfuran	625-86-5	96	13.37	<0.001
C ₉ H ₁₄ O	2-Pentylfuran	3777-69-3	138	24.93	<0.001
Nitrogenated compounds					
N ₂	Nitrogen	7727-37-9	28	1.77	1.140
H ₃ N	Ammonia	7664-41-7	17	2.96	0.046
C ₂ H ₃ N	Acetonitrile	75-05-8	41	6.84	0.010
C ₃ H ₅ N	Propargylamine	2450-71-7	55	9.26	<0.001
C ₄ H ₅ N	Pyrrole	109-97-7	67	14.14	0.001
C ₅ H ₅ N	Pyridine	110-86-1	79	15.27	<0.001
C ₂ H ₅ NO	Acetamide	60-35-5	59	16.39	0.004
C ₃ H ₅ NO ₂	2-Oxo-propionamide	x	87	17.19	0.002
C ₆ H ₉ N	2,3-Dimethyl-1H-pyrrole	600-28-2	95	17.94	<0.001
C ₆ H ₇ N	2-Methylpyridine	109-06-8	93	18.42	<0.001
C ₆ H ₇ N	3-Methylpyridine	108-99-6	93	20.15	<0.001
C ₄ H ₅ NO ₂	Succinimide	123-56-8	99	28.58	0.002
C ₆ H ₁₃ NO	Hexanamide	628-02-4	115	30.47	0.001
C ₇ H ₁₅ NO	Heptanamide	628-62-6	129	33.57	<0.001
C ₈ H ₁₇ NO	Octanamide	629-01-6	143	37.29	0.001
C ₉ H ₁₉ NO	Nonanamide	1120-07-6	157	42.63	0.001
C ₈ H ₁₃ NO	4-Cyclopropyl-4-methylpyrrolidin-2-one	(461078)	139	49.89	0.002
C ₁₀ H ₂₁ NO	Decanamide	2319-29-1	171	50.89	0.002
C ₁₂ H ₂₅ NO	Dodecanamide	1120-16-7	199	84.18	0.001
Sulfonated compounds					
H ₂ S	Hydrogen sulfide	7783-06-4	34	2.76	0.014
COS	Carbonyl sulfide	463-58-1	60	3.31	0.002

O ₂ S	Sulfur dioxide	7446-09-5	64	4.61	0.217
CH ₄ S	Methanethiol	74-93-1	48	5.38	0.002
CS ₂	Carbon disulfide	75-15-0	76	7.51	0.004
C ₄ H ₄ S	Thiophene	110-02-1	84	11.74	<0.001
C ₂ H ₆ S ₂	Dimethyl disulfide	624-92-0	94	14.67	<0.001
C ₅ H ₆ S	2-Methylthiophene	554-14-3	98	15.74	0.001
C ₅ H ₆ S	3-Methylthiophene	616-44-4	98	16.09	0.001
C ₁₀ H ₁₆ S	2-Hexylthiophene	18794-77-9	168	33.74	0.001
Inorganic compounds					
<i>Oxides</i>					
CO ₂	Carbon dioxide	124-38-9	44	1.95	1.484
H ₂ O	Water	7732-18-5	18	3.16	89.515
<i>Noble gases</i>					
Ar	Argon	7440-37-1	40	1.72	0.006

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).