Table S3. Results of GC–MS analysis of volatiles extracted by mechanical shock crushing from arsenopyrite (Blagodatnoye deposit, Yenisei ridge).

| Formula | Name | [1]CAS | [2]MW | Arsenopyrite 7/96.0 | |
|---|---|---|---|---|---|
| | | | | [3]RT, min | [4]A, % |
| **Aliphatic hydrocarbons** | | | | | |
| *Paraffins* | | | | | |
| $CH_4$ | Methane | 74-82-8 | 16 | 1.72 | 1.513 |
| $C_2H_6$ | Ethane | 74-84-0 | 30 | 2.45 | 0.020 |
| $C_6H_{14}$ | n-Hexane | 110-54-3 | 86 | 12.02 | 0.009 |
| $C_7H_{16}$ | n-Heptane | 142-82-5 | 100 | 16.07 | 0.008 |
| $C_8H_{18}$ | n-Octane | 111-65-9 | 114 | 20.17 | 0.009 |
| $C_9H_{20}$ | n-Nonane | 111-84-2 | 128 | 24.03 | 0.011 |
| $C_{10}H_{22}$ | n-Decane | 124-18-5 | 142 | 27.63 | 0.007 |
| $C_{11}H_{24}$ | n-Undecane | 1120-21-4 | 156 | 30.96 | 0.011 |
| $C_{12}H_{26}$ | n-Dodecane | 112-40-3 | 170 | 34.09 | 0.006 |
| $C_{13}H_{28}$ | n-Tridecane | 629-50-5 | 184 | 38.09 | 0.013 |
| $C_{13}H_{28}$ | 6-Methyldodecane | 6044-71-9 | 184 | 35.45 | 0.020 |
| $C_{14}H_{30}$ | n-Tetradecane | 629-59-4 | 198 | 44.23 | 0.318 |
| $C_{15}H_{32}$ | n-Pentadecane | 629-62-9 | 212 | 50.77 | 0.036 |
| $C_{16}H_{34}$ | 7-Methylpentadecane | 6165-40-8 | 226 | 53.62 | 0.025 |
| $C_{16}H_{34}$ | n-Hexadecane | 544-76-3 | 226 | 68.59 | 0.030 |
| $C_{17}H_{36}$ | 7-Methylhexadecane | 26730-20-1 | 240 | 75.34 | 0.078 |
| $C_{17}H_{36}$ | n-Heptadecane | 629-78-7 | 240 | 93.19 | 0.040 |
| $C_{18}H_{38}$ | 3-Methylheptadecane | 6418-44-6 | 254 | 114.97 | 0.083 |
| *Olefins* | | | | | |
| $C_4H_8$ | 2-Methyl-1-propene | 115-11-7 | 56 | 5.93 | 0.500 |
| $C_4H_8$ | 2-Butene | 107-01-7 | 56 | 6.15 | 0.371 |
| $C_5H_{10}$ | 2-Methyl-2-butene | 513-35-9 | 70 | 8.31 | 0.002 |
| $C_5H_8$ | 1,3-Pentadiene | 1574-41-0 | 68 | 8.54 | 0.091 |
| $C_5H_8$ | (E)-1,3-Pentadiene | 2004-70-8 | 68 | 8.66 | 0.010 |
| $C_5H_8$ | (Z)-1,3-Pentadiene | 1574-41-0 | 68 | 8.96 | <0.001 |
| $C_6H_{12}$ | 1-Hexene | 592-41-6 | 84 | 11.69 | 0.004 |
| $C_6H_{12}$ | 2,3-Dimethyl-2-butene | 563-79-1 | 84 | 13.57 | 0.002 |
| $C_7H_{14}$ | 1-Heptene | 592-76-7 | 98 | 15.70 | 0.004 |
| $C_8H_{16}$ | 3-Ethyl-2-methyl-2-pentene | 19780-67-7 | 112 | 19.38 | 0.006 |
| $C_8H_{16}$ | 2,3-Dimethyl-2-hexene | 7145-20-2 | 112 | 19.52 | 0.014 |
| $C_8H_{16}$ | 1-Octene | 111-66-0 | 112 | 19.82 | 0.028 |
| $C_8H_{16}$ | (Z)-3-Octene | 14850-22-7 | 112 | 19.93 | 0.022 |
| $C_8H_{16}$ | (E)-2-Octene | 13389-42-9 | 112 | 20.03 | 0.010 |
| $C_8H_{16}$ | (Z)-2-Octene | 7642-04-8 | 112 | 20.28 | 0.006 |
| $C_9H_{18}$ | 1-Nonene | 124-11-8 | 126 | 23.70 | 0.004 |
| $C_{10}H_{20}$ | 1-Decene | 872-05-9 | 140 | 27.36 | 0.003 |
| $C_{11}H_{22}$ | 1-Undecene | 821-95-4 | 154 | 30.74 | 0.001 |

| | | | | | |
|---|---|---|---|---|---|
| $C_{12}H_{24}$ | 1-Dodecene | 112-41-4 | 168 | 33.96 | 0.002 |
| $C_{13}H_{26}$ | 1-Tridecene | 2437-56-1 | 182 | 37.79 | 0.001 |
| **Cyclic hydrocarbons** | | | | | |
| *Cycloalkanes (naphthenes) and cycloalkenes* | | | | | |
| $C_5H_{10}$ | Cyclopentane | 287-92-3 | 70 | 8.68 | 0.051 |
| $C_6H_{12}$ | Cyclohexane | 110-82-7 | 84 | 15.74 | 0.006 |
| *Arenes* | | | | | |
| $C_6H_6$ | Benzene | 71-43-2 | 78 | 12.59 | 0.046 |
| $C_7H_8$ | Toluene | 108-88-3 | 92 | 17.04 | 0.025 |
| $C_7H_7F$ | (Fluoromethyl)benzene | 350-50-5 | 110 | 20.72 | 0.001 |
| $C_8H_{10}$ | Ethylbenzene | 100-41-4 | 106 | 21.08 | 0.013 |
| $C_8H_{10}$ | p-Xylene | 106-42-3 | 106 | 21.35 | 0.050 |
| $C_8H_{10}$ | o-Xylene | 95-47-6 | 106 | 21.55 | 0.006 |
| $C_8H_8$ | Styrene | 100-42-5 | 104 | 22.00 | 0.001 |
| $C_8H_{10}$ | m-Xylene | 108-38-3 | 106 | 22.02 | 0.010 |
| $C_9H_{12}$ | Propylbenzene | 103-65-1 | 120 | 24.91 | 0.029 |
| $C_9H_{12}$ | 1-Ethyl-3-methylbenzene | 620-14-4 | 120 | 25.11 | 0.003 |
| $C_9H_{12}$ | 1-Ethyl-4-methylbenzene | 622-96-8 | 120 | 25.90 | 0.015 |
| $C_9H_{12}$ | 1-Ethyl-2-methylbenzene | 611-14-3 | 120 | 26.69 | 0.020 |
| $C_{10}H_{14}$ | o-Cymene | 527-84-4 | 134 | 27.74 | 0.002 |
| $C_{10}H_{14}$ | Butylbenzene | 104-51-8 | 134 | 28.68 | 0.048 |
| $C_{11}H_{16}$ | Pentylbenzene | 538-68-1 | 148 | 32.09 | 0.045 |
| $C_{12}H_{18}$ | Hexylbenzene | 1077-16-3 | 162 | 35.52 | 0.023 |
| $C_{13}H_{20}$ | Heptylbenzene | 1078-71-3 | 176 | 40.40 | 0.011 |
| $C_{14}H_{22}$ | Octylbenzene | 2189-60-8 | 190 | 47.93 | 0.015 |
| $C_{15}H_{24}$ | Nonylbenzene | 1081-77-2 | 204 | 59.65 | 0.014 |
| *Polycyclic aromatic hydrocarbons (PAH)* | | | | | |
| $C_{10}H_8$ | Naphthalene | 91-20-3 | 128 | 32.24 | 0.004 |
| $C_{11}H_{10}$ | 1-Methylnaphthalene | 90-12-0 | 142 | 36.09 | 0.003 |
| $C_{11}H_{10}$ | 2-Methylnaphthalene | 91-57-6 | 142 | 36.59 | 0.003 |
| **Oxygenated hydrocarbons** | | | | | |
| *Alcohols* | | | | | |
| $CH_4O$ | Methanol | 67-56-1 | 32 | 4.90 | 0.136 |
| $C_2H_6O$ | Ethanol | 64-17-5 | 46 | 6.48 | 0.006 |
| $C_3H_8O$ | Isopropyl Alcohol | 67-63-0 | 60 | 8.06 | 0.001 |
| $C_3H_8O$ | 1-Propanol | 71-23-8 | 60 | 9.11 | 0.002 |
| $C_4H_{10}O$ | 1-Butanol | 71-36-3 | 74 | 12.86 | 0.085 |
| $C_6H_6O$ | Phenol | 108-95-2 | 94 | 24.75 | 0.003 |
| $C_8H_{16}O$ | 4-Ethylcyclohexanol | 4534-74-1 | 128 | 28.03 | 0.002 |
| *Ethers and esters* | | | | | |
| $C_5H_8O_2$ | Methyl methacrylate | 80-62-6 | 100 | 14.49 | <0.001 |
| $C_6H_{12}O$ | Tetrahydro-3-methyl-2H-pyran | 26093-63-0 | 100 | 17.67 | 0.002 |
| $C_8H_{14}O_2$ | γ-Octalactone | 104-50-7 | 142 | 34.55 | 0.001 |

| | | | | | |
|---|---|---|---|---|---|
| $C_9H_{16}O_2$ | γ-Nonalactone | 104-61-0 | 156 | 38.34 | 0.001 |
| $C_{13}H_{26}O_2$ | 1-Methylethyl ester decanoic acid | 2311-59-3 | 214 | 44.71 | 0.283 |
| *Aldehydes* | | | | | |
| $C_2H_4O$ | Acetaldehyde | 75-07-0 | 44 | 5.26 | 0.121 |
| $C_3H_4O$ | 2-Propenal | 107-02-8 | 56 | 7.29 | 0.003 |
| $C_3H_6O$ | n-Propanal | 123-38-6 | 58 | 7.46 | 0.018 |
| $C_4H_6O$ | 2-Methyl-2-propenal | 78-85-3 | 70 | 9.74 | 0.014 |
| $C_4H_8O$ | 2-Methyl-propanal | 78-84-2 | 72 | 9.76 | 0.002 |
| $C_4H_8O$ | n-Butanal | 123-72-8 | 72 | 10.54 | 0.025 |
| $C_5H_8O$ | (E)-2-Methyl-2-butenal | 497-03-0 | 84 | 13.42 | 0.007 |
| $C_5H_{10}O$ | 3-Methylbutanal | 590-86-3 | 86 | 13.67 | 0.055 |
| $C_5H_{10}O$ | n-Pentanal | 110-62-3 | 86 | 14.69 | 0.005 |
| $C_5H_4O_2$ | Furfural | 98-01-1 | 96 | 17.45 | <0.001 |
| $C_6H_{10}O$ | 2-Methyl-2-pentenal | 623-36-9 | 98 | 18.12 | 0.001 |
| $C_5H_4O_2$ | 3-Furaldehyde | 498-60-2 | 96 | 18.32 | 0.002 |
| $C_6H_{12}O$ | n-Hexanal | 66-25-1 | 100 | 19.00 | 0.035 |
| $C_7H_{14}O$ | n-Heptanal | 111-71-7 | 114 | 23.26 | 0.005 |
| $C_6H_6O_2$ | 5-Methyl-2-furancarboxaldehyde | 620-02-0 | 110 | 23.38 | <0.001 |
| $C_7H_6O$ | Benzaldehyde | 100-52-7 | 106 | 24.11 | 0.008 |
| $C_8H_{16}O$ | 2-Ethylhexanal | 123-05-7 | 128 | 25.60 | 0.007 |
| $C_8H_{16}O$ | n-Octanal | 124-13-0 | 128 | 26.96 | 0.005 |
| $C_9H_{18}O$ | n-Nonanal | 124-19-6 | 142 | 30.46 | 0.005 |
| $C_{10}H_{20}O$ | n-Decanal | 112-31-2 | 156 | 33.71 | 0.006 |
| $C_{11}H_{22}O$ | n-Undecanal | 112-44-7 | 170 | 37.65 | 0.003 |
| $C_{12}H_{24}O$ | n-Dodecanal | 112-54-9 | 184 | 43.53 | <0.001 |
| *Ketones* | | | | | |
| $C_3H_6O$ | 2-Propanone | 67-64-1 | 58 | 7.63 | 0.022 |
| $C_4H_6O_2$ | 2,3-Butanedione | 431-03-8 | 86 | 10.63 | <0.001 |
| $C_4H_8O$ | 2-Butanone | 78-93-3 | 72 | 10.71 | 0.004 |
| $C_5H_{10}O$ | 2-Pentanone | 107-87-9 | 86 | 14.45 | <0.001 |
| $C_6H_{12}O$ | 2-Hexanone | 591-78-6 | 100 | 18.75 | 0.002 |
| $C_7H_{14}O$ | 2-Heptanone | 110-43-0 | 114 | 22.85 | 0.005 |
| $C_9H_{18}O$ | 2-Nonanone | 821-55-6 | 142 | 30.14 | 0.002 |
| $C_{10}H_{20}O$ | 2-Decanone | 693-54-9 | 156 | 33.36 | 0.004 |
| $C_8H_4O_3$ | 1,3-Isobenzofurandione | 85-44-9 | 148 | 35.97 | 0.014 |
| $C_{11}H_{22}O$ | 2-Undecanone | 53452-70-3 | 170 | 37.09 | 0.005 |
| $C_{15}H_{30}O$ | 2-Pentadecanone | 2345-28-0 | 226 | 87.49 | 0.022 |
| *Carboxylic acids* | | | | | |
| $C_2H_4O_2$ | Acetic acid | 64-19-7 | 60 | 11.44 | 0.027 |
| $C_3H_6O_2$ | n-Propanoic acid | 79-09-4 | 74 | 15.49 | 0.001 |
| $C_4H_8O_2$ | n-Butanoic acid | 107-92-6 | 88 | 19.13 | 0.010 |
| $C_5H_{10}O_2$ | 3-Methylbutanoic acid | 503-74-2 | 102 | 22.10 | 0.003 |
| $C_5H_{10}O_2$ | n-Pentanoic acid | 109-52-4 | 102 | 23.06 | 0.002 |

| | | | | | |
|---|---|---|---|---|---|
| $C_6H_{12}O_2$ | n-Hexanoic acid | 142-62-1 | 116 | 26.54 | 0.025 |
| $C_7H_{14}O_2$ | n-Heptanoic acid | 111-14-8 | 130 | 30.01 | 0.004 |
| $C_8H_{16}O_2$ | n-Octanoic acid | 124-07-2 | 144 | 32.96 | 0.120 |
| $C_9H_{18}O_2$ | n-Nonanoic acid | 112-05-0 | 158 | 36.60 | 0.009 |
| $C_{10}H_{20}O_2$ | n-Decanoic acid | 334-48-5 | 172 | 41.73 | 0.078 |
| $C_{12}H_{24}O_2$ | n-Dodecanoic acid | 143-07-7 | 200 | 62.12 | 0.312 |
| $C_{14}H_{28}O_2$ | n-Tetradecanoic acid | 544-63-8 | 228 | 117.63 | 0.087 |
| **Heterocyclic compounds** | | | | | |
| *Furans* | | | | | |
| $C_5H_6O$ | 2-Methylfuran | 534-22-5 | 82 | 10.31 | 0.001 |
| $C_5H_6O$ | 3-Methylfuran | 930-27-8 | 82 | 10.59 | <0.001 |
| $C_6H_8O$ | 2-Ethylfuran | 3208-16-0 | 96 | 14.57 | <0.001 |
| $C_9H_{14}O$ | 2-Pentylfuran | 3777-69-3 | 138 | 26.10 | 0.001 |
| **Nitrogenated compounds** | | | | | |
| $N_2$ | Nitrogen | 7727-37-9 | 28 | 1.62 | 0.367 |
| $C_2H_3N$ | Acetonitrile | 75-05-8 | 41 | 6.88 | 0.007 |
| $C_4H_5NO_2$ | Succinimide | 123-56-8 | 99 | 28.86 | 0.002 |
| **Sulfonated compounds** | | | | | |
| $H_2S$ | Hydrogen sulfide | 7783-06-4 | 34 | 2.90 | 0.005 |
| COS | Carbonyl sulfide | 463-58-1 | 60 | 3.45 | 0.011 |
| $O_2S$ | Sulfur dioxide | 7446-09-5 | 64 | 4.46 | 2.371 |
| $CS_2$ | Carbon disulfide | 75-15-0 | 76 | 7.76 | 0.048 |
| $C_4H_4S$ | Thiophene | 110-02-1 | 84 | 12.32 | 0.021 |
| $C_2H_6S_2$ | Dimethyl disulfide | 624-92-0 | 94 | 15.37 | <0.001 |
| $C_5H_6S$ | 2-Methylthiophene | 554-14-3 | 98 | 16.54 | 0.007 |
| $C_5H_6S$ | 3-Methylthiophene | 616-44-4 | 98 | 16.89 | 0.117 |
| $C_8H_{12}S$ | 2-(1,1-Dimethylethyl)-thiophene | 1689-78-7 | 140 | 27.13 | 0.001 |
| $C_8H_{12}S$ | 3-(1,1-Dimethylethyl)-thiophene | 1689-79-8 | 140 | 28.24 | 0.004 |
| **Inorganic compounds** | | | | | |
| *Oxides* | | | | | |
| $CO_2$ | Carbon dioxide | 124-38-9 | 44 | 1.93 | 1.529 |
| $H_2O$ | Water | 7732-18-5 | 18 | 3.21 | 90.140 |
| *Noble gases* | | | | | |
| Ar | Argon | 7440-37-1 | 40 | 1.58 | 0.001 |

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