

# Chemical Diversity of Metal Sulfide Minerals and its Implications for Origin of Life

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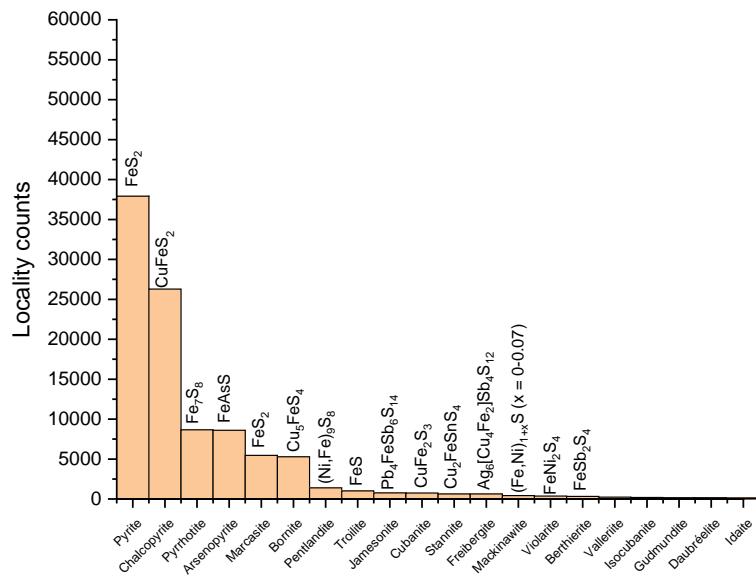


Figure S1. Species-locality distribution of Fe-containing sulfides (top 20).

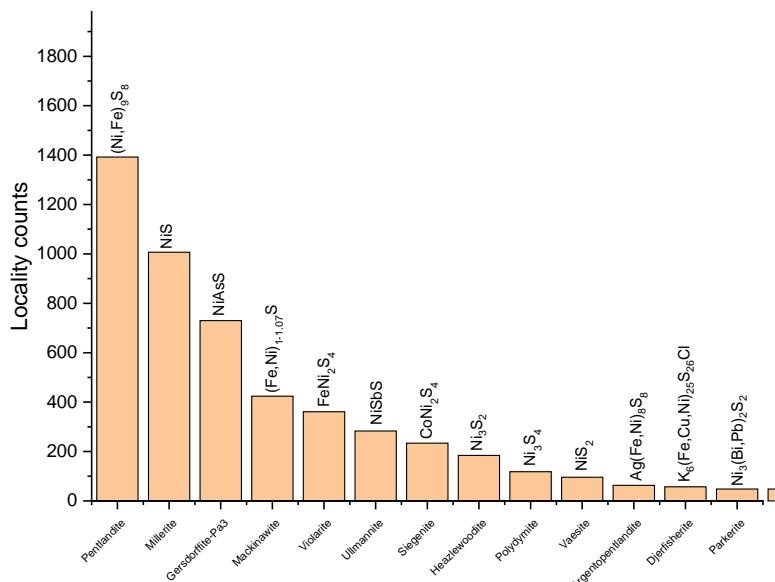
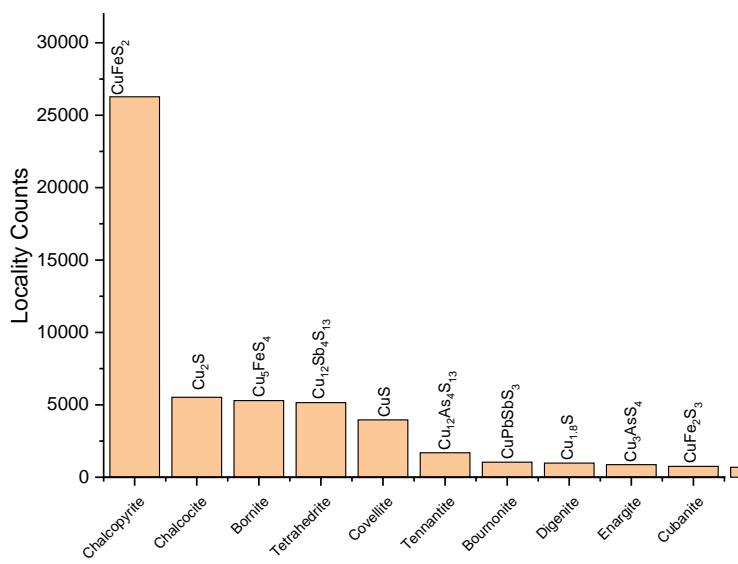
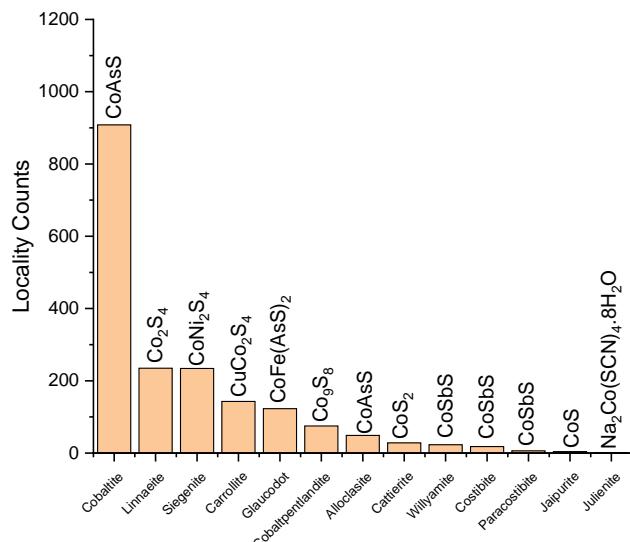


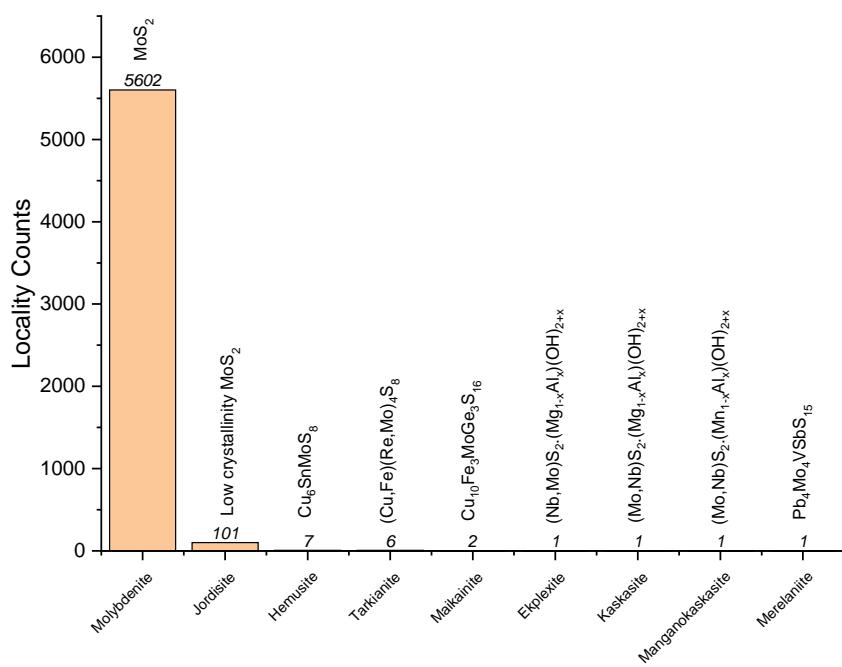
Figure S2. Species-locality distribution of Ni-containing sulfides (top 12).



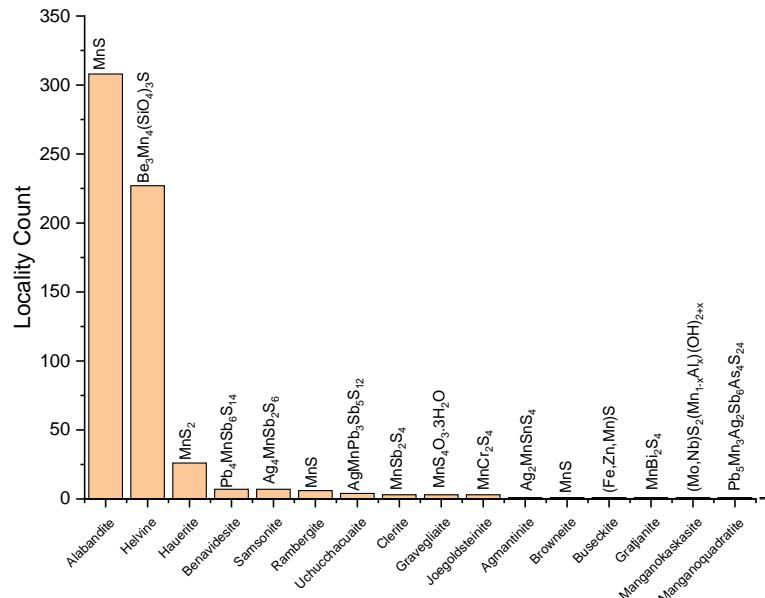
**Figure S3.** Species-locality distribution of Cu-containing sulfides (top 10).



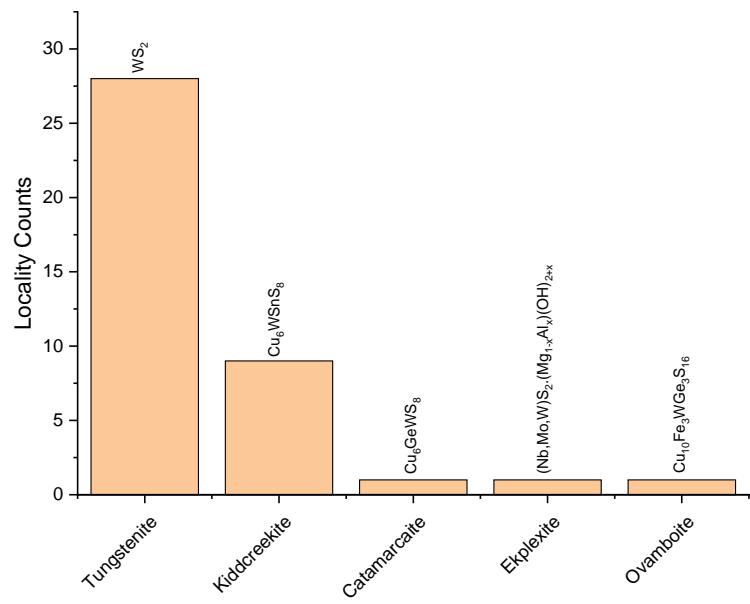
**Figure S4.** Species-locality distribution of Co-containing sulfides.



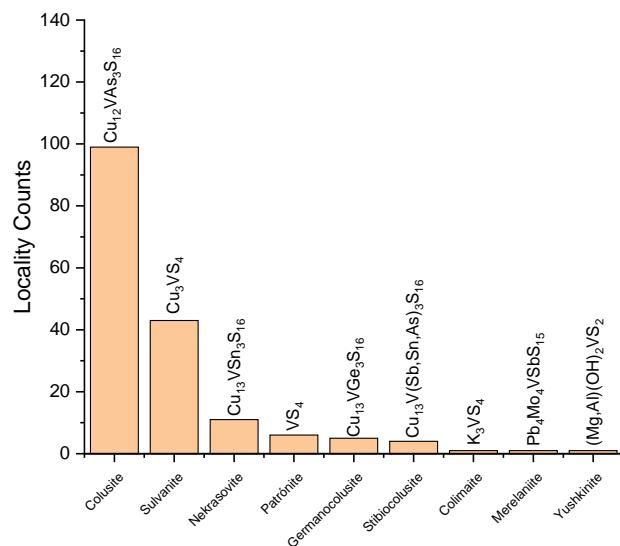
**Figure S5.** Species-locality distribution of Mo-containing sulfides.



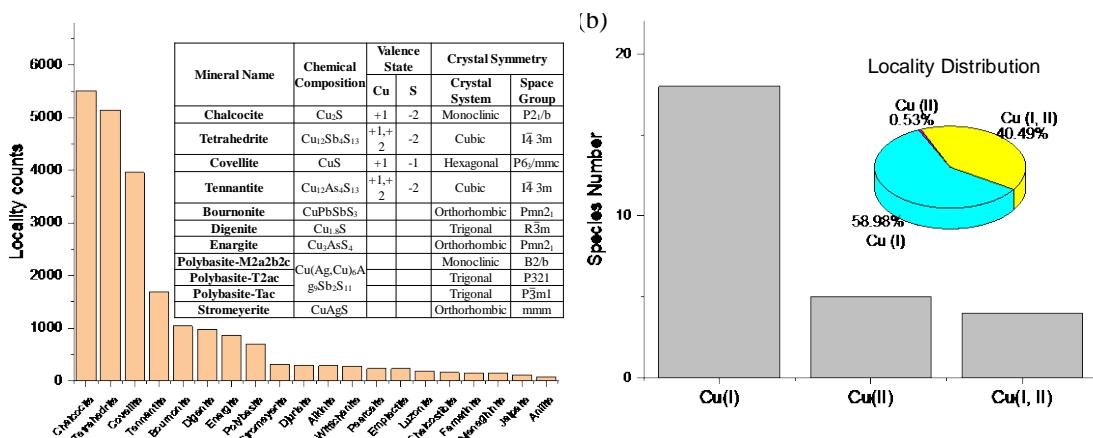
**Figure S6.** Species-locality distribution of Mn-containing sulfides.



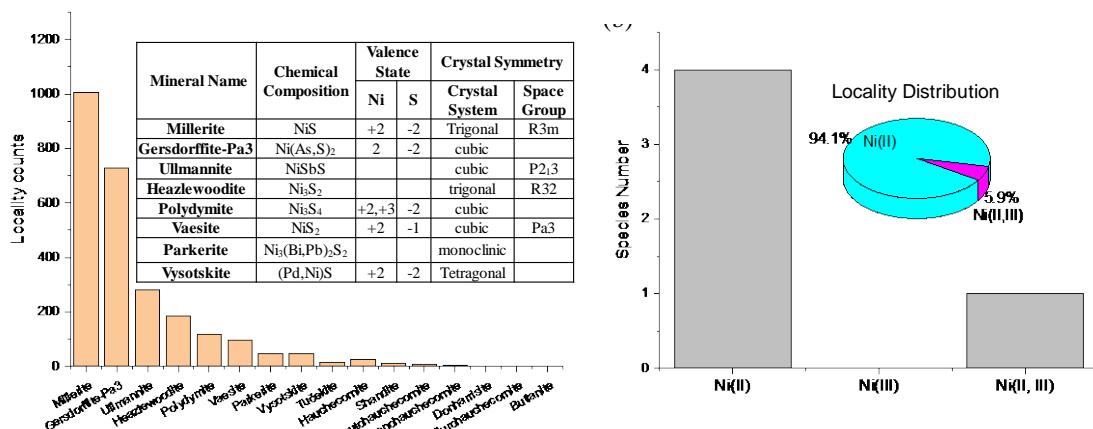
**Figure S7.** Species-locality distribution of W-containing sulfides.



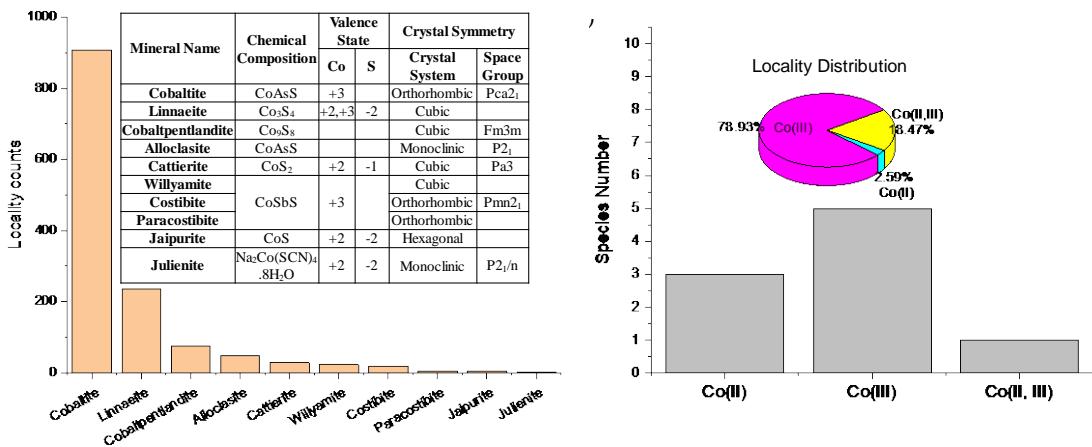
**Figure S8.** Species-locality distribution of V-containing sulfides.



**Figure S9.** (a) Locality-mineral distribution of Cu mono-metal sulfide species and chemical diversity with regards to chemical composition, Cu/S valence states and crystal symmetry; (b) plots of the distribution of species type and locality counts for species containing Cu(I), Cu(II) and Cu(I,II) valence states.



**Figure S10.** (a) Locality-mineral distribution of Ni mono-metal sulfide species and chemical diversity with regards to chemical composition, Ni/S valence states and crystal symmetry; (b) plots of the distribution of species type and locality counts for species containing Ni(II), Ni(III) and Ni(II,III) valence states.



**Figure S11.** (a) Locality-mineral distribution of Co mono-metal sulfide species and chemical diversity with regards to chemical composition, Co/S valence states and crystal symmetry; (b) plots of the distribution of species type and locality counts for species containing Co(II), Co(III) and Co(II,III) valence states.

**Table S1.** Chemical properties of Fe-Cu and Fe-Ni binary metal sulfide minerals.

Mineral Name	Locality Counts	Chemical Composition	Fe, Cu			Crystal System	Space Group
			Cu	Fe	S		
Chalcopyrite	26279	CuFeS <sub>2</sub>	+1	+3	-2	Tetragonal	I42d
Bornite	5293	Cu <sub>5</sub> FeS <sub>4</sub>	+1	+3	-2	Orthorhombic	Pbca
Cubanite	748	CuFe <sub>2</sub> S <sub>3</sub>	+1	+2,+3	-2	Orthorhombic	2/m2/m2/m
Stannite	632	Cu <sub>2</sub> FeSn <sub>4</sub> S <sub>4</sub>	+1	+2	-2	Tetragonal	I42m
Freibergite	630	Ag <sub>6</sub> Cu <sub>4</sub> Fe <sub>2</sub> Sb <sub>4</sub> S <sub>12</sub>	+1	+2	-2	Tetragonal	I43m
Vallerite	229	2[(Fe,Cu)S]·1.53[(Mg,Al)(OH) <sub>2</sub> ]	+2	+2	-2	Hexagonal	-
Isocubanite	184	CuFe <sub>2</sub> S <sub>3</sub>	+1	+2,+3	-2	Cubic	Fm3m
Idaite	133	Cu <sub>3</sub> FeS <sub>4</sub>	+2	+2	-2	Hexagonal	-

Mineral Name	Locality Counts	Chemical Composition	Fe, Ni			Crystal System	Space Group
			Fe	Ni	S		
Pentlandite	1392	(Ni,Fe) <sub>9</sub> S <sub>8</sub>	-	-	-	Cubic	Fm3m
Mackinawite	424	(Fe,Ni) <sub>1+x</sub> S (x = 0-0.07)	+2	+2	-2	Tetragonal	P4/nmm
Violarite	361	FeNi <sub>2</sub> S <sub>4</sub>	+2	+3	-2	Cubic	-
Smythite	71	(Fe,Ni) <sub>3+x</sub> S <sub>4</sub> (x ≈ 0-0.3)	-	-	-	Trigonal	R <sub>3</sub> m
Argentopentlandite	63	Ag(Fe,Ni) <sub>8</sub> S <sub>8</sub>	-	-	-	Cubic	Fm3m
Godlevskite	32	(Ni,Fe) <sub>9</sub> S <sub>8</sub>	-	-	-	Orthorhombic	C222

**Table S2.** Sulfide minerals with ternary metal compositions.

Mineral Name	Locality Counts	Chemical Composition
Djerfisherite	57	K <sub>6</sub> (Fe,Cu,Ni) <sub>25</sub> S <sub>26</sub> Cl
Sugakiite	3	Cu(Fe,Ni) <sub>8</sub> S <sub>8</sub>
Kharaelakhite	2	(Cu,Pt,Pb,Fe,Ni) <sub>9</sub> S <sub>8</sub>
Owensite	2	(Ba,Pb <sup>2+</sup> ) <sub>6</sub> (Cu <sup>1+</sup> ,Fe <sup>2+</sup> ,Ni <sup>2+</sup> ) <sub>25</sub> S <sub>2-27</sub>
Samaniite	2	Cu <sub>2</sub> Fe <sub>5</sub> Ni <sub>2</sub> S <sub>8</sub>
Ferhodsrite	1	(Fe,Rh,Ni,Ir,Cu,Pt) <sub>9</sub> S <sub>8</sub>
Zoharite	1	(Ba,K) <sub>6</sub> (Fe,Cu,Ni) <sub>25</sub> S <sub>27</sub>
Tarkianite	6	(Cu,Fe)(Re,Mo) <sub>4</sub> S <sub>8</sub>
Maikainite	2	Cu <sup>1+10</sup> Fe <sup>2+3</sup> Mo <sup>4+</sup> Ge <sup>4+3</sup> S <sup>2-16</sup>
Ovamboite	1	Cu <sup>1+10</sup> Fe <sup>2+3</sup> W <sup>4+</sup> Ge <sup>4+3</sup> S <sup>2-16</sup>

**Table S3.** X-ray amorphous mineral species in the RRUFF database.

Mineral Name	Chemical Composition
Delvauxite	CaFe <sup>3+4</sup> (P <sup>5+</sup> O <sub>4</sub> ) <sub>2</sub> (OH) <sub>8</sub> . 4-5H <sub>2</sub> O
Diadochite	Fe <sup>3+2</sup> (PO <sub>4</sub> )(SO <sub>4</sub> )(OH). 6H <sub>2</sub> O
Ekanite	Ca <sub>2</sub> ThSi <sub>8</sub> O <sub>20</sub>
Evansite	Al <sub>3</sub> PO <sub>4</sub> (OH) <sub>6</sub> . 8H <sub>2</sub> O
Georgeite	Cu <sup>2+2</sup> CO <sub>3</sub> (OH) <sub>2</sub>
Ice	H <sub>2</sub> O
Jordisite	Mo <sup>4+</sup> S <sup>2-2</sup>
Zaratite	Ni <sup>2+3</sup> C <sup>4+</sup> O <sub>3</sub> (OH) <sub>4</sub> . 4H <sub>2</sub> O