Chemical Diversity of Metal Sulfide Minerals and its Implications for Prebiotic Catalysis

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

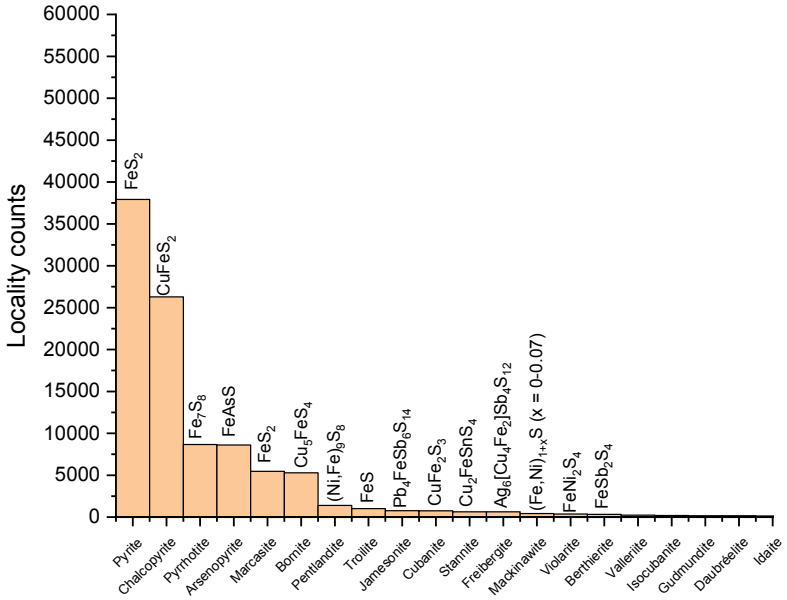


Figure S2 Species-locality distribution of Ni-containing sulfides (top 12)

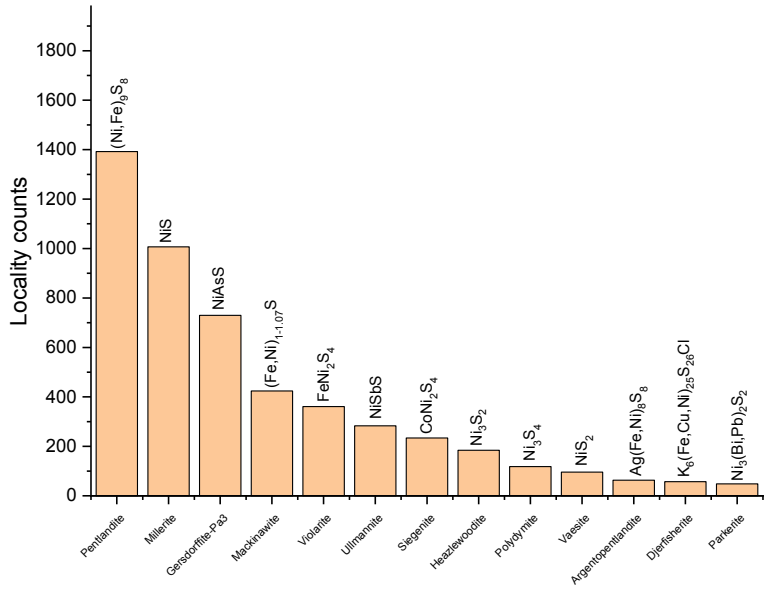


Figure S3 Species-locality distribution of Cu-containing sulfides (top 10)

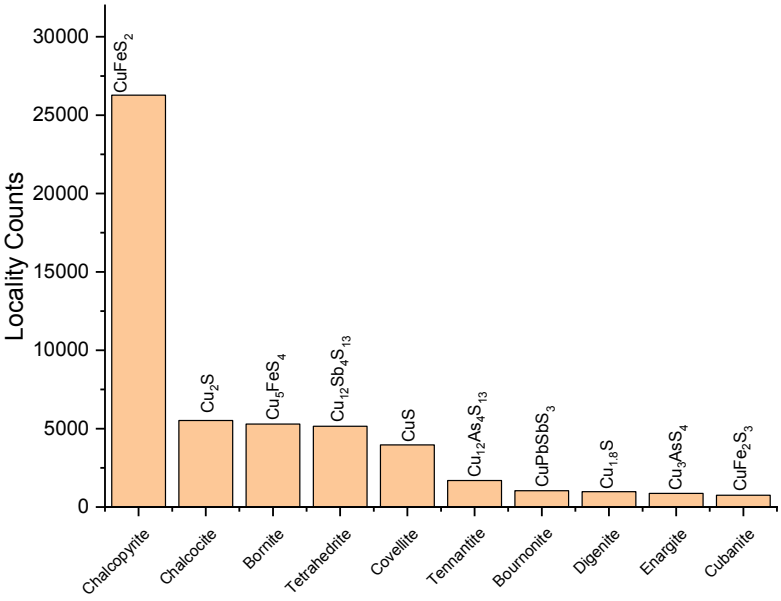


Figure S4 Species-locality distribution of Co-containing sulfides

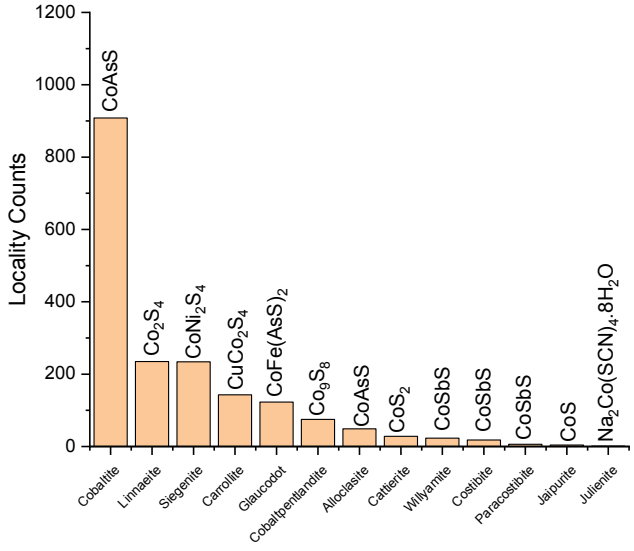


Figure S5 Species-locality distribution of Mo-containing sulfides

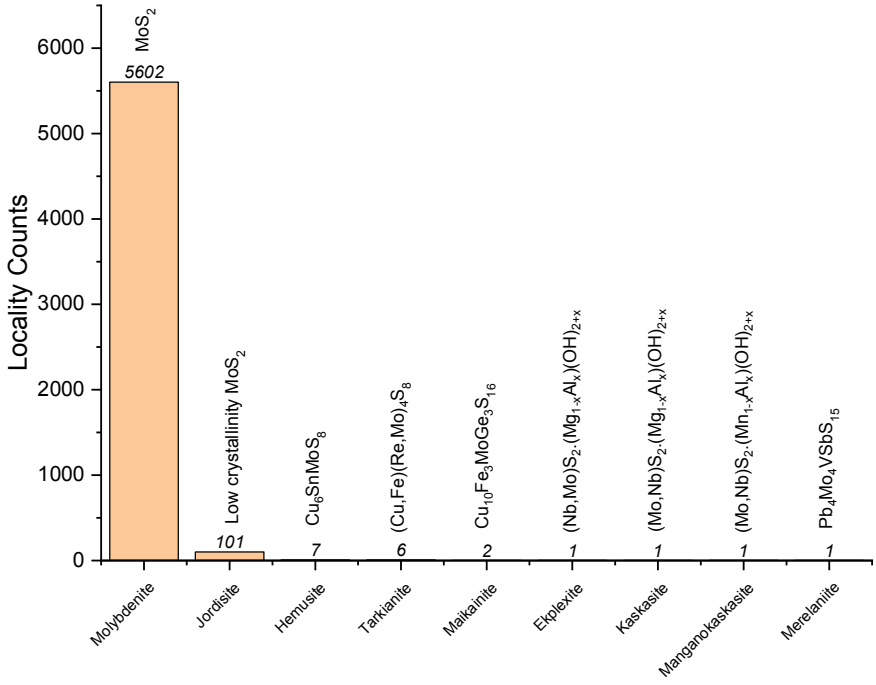


Figure S6 Species-locality distribution of Mn-containing sulfides

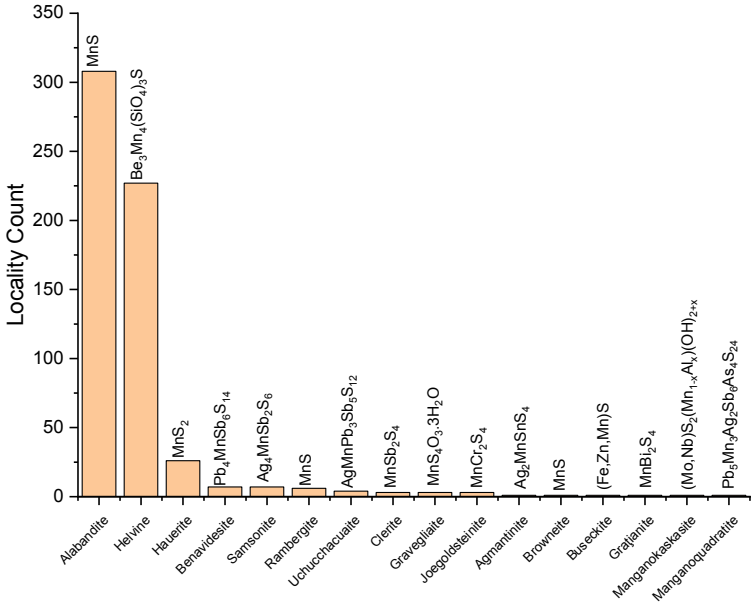


Figure S7 Species-locality distribution of W-containing sulfides

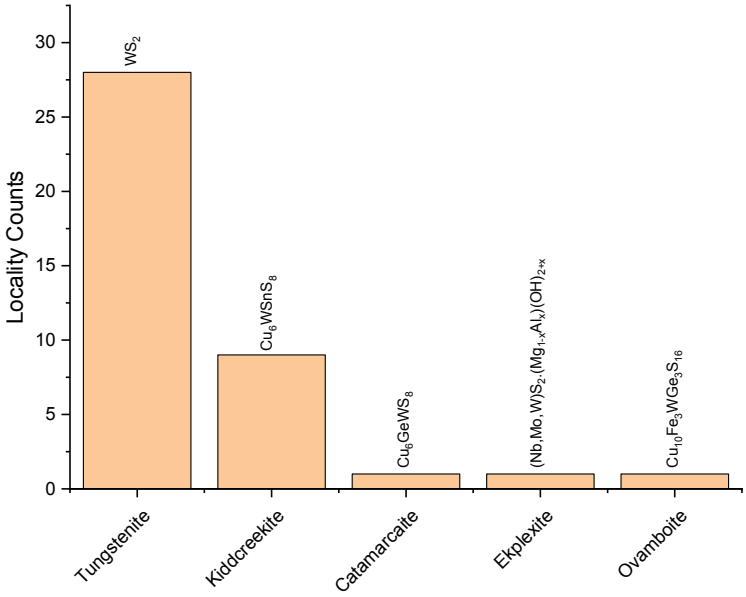


Figure S8 Species-locality distribution of V-containing sulfides

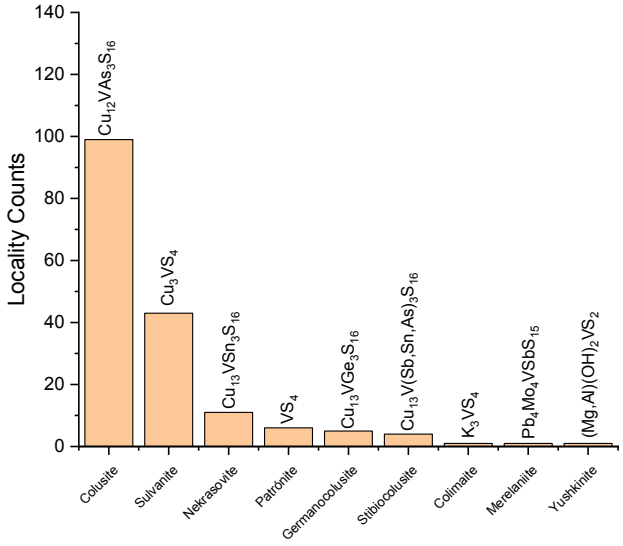
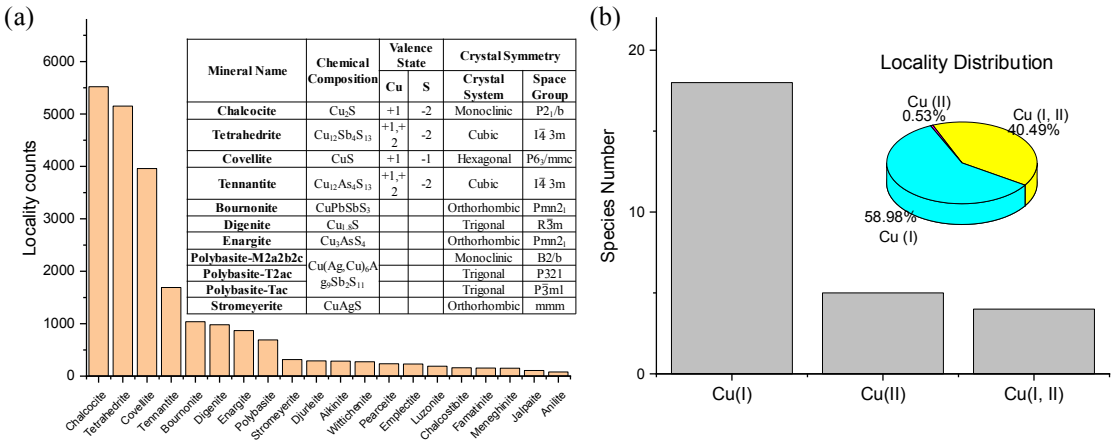
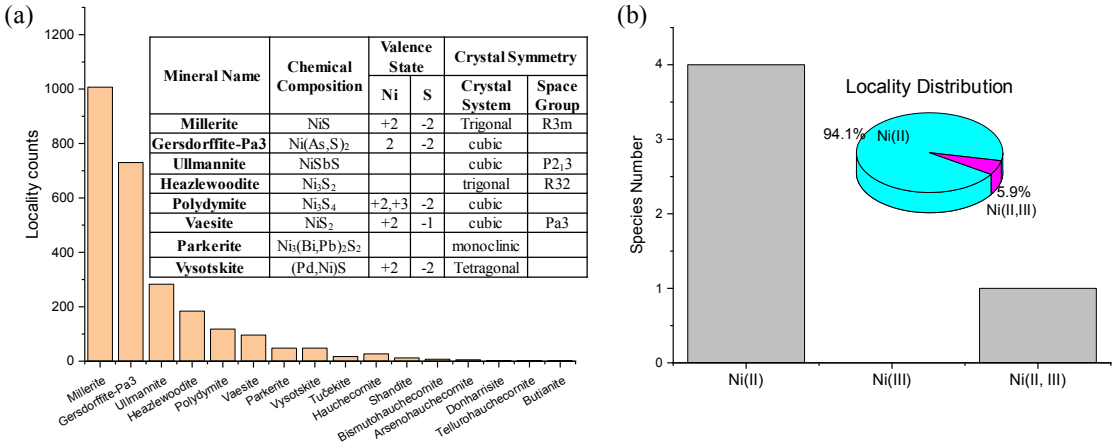


Figure S9 (a) Locality-mineral distribution of Cu mono-metal sulfide species and chemical diversity with regards to chemical composition, Cu/S valence states and crystal symmetry; (b) plots of the distribution of species type and locality counts for species containing Cu(I), Cu(II) and Cu(I,II) valence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



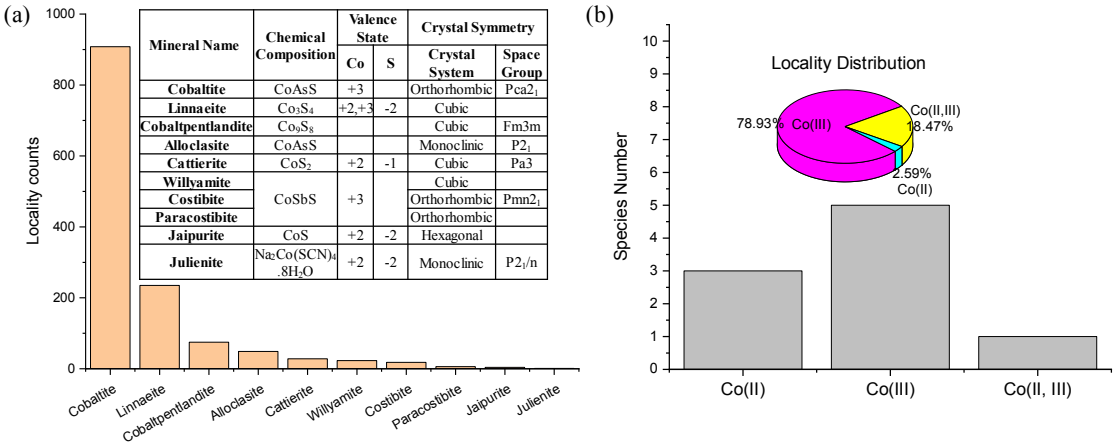
Mineral Name	Chemical Composition	Valence State		Crystal Symmetry	
		Cu	S	Crystal System	Space Group
Chalcocite	Cu_2S	+1	-2	Monoclinic	$P2_1/b$
Tetrahedrite	$Cu_{12}Sb_4S_{13}$	+1,+2	-2	Cubic	$I\bar{4}\ 3m$
Covellite	CuS	+1	-1	Hexagonal	$P6_3/mmc$
Tennantite	$Cu_{12}As_4S_{13}$	+1,+2	-2	Cubic	$I\bar{4}\ 3m$
Bournonite	$CuPbSbS_3$			Orthorhombic	$Pmn2_1$
Digenite	$Cu_{1.8}S$			Trigonal	$R\bar{3}m$
Enargite	Cu_3AsS_4			Orthorhombic	$Pmn2_1$
Polybasite-M2a2b2c	$Cu(Ag,Cu)_6Ag_9Sb_2S_{11}$			Monoclinic	B2/b
Polybasite-T2ac				Trigonal	P321
Polybasite-Tac				Trigonal	$P\bar{3}m1$
Stromeyerite	CuAgS			Orthorhombic	mmm

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.



Mineral Name	Chemical Composition	Valence State		Crystal Symmetry	
		Ni	S	Crystal System	Space Group
Millerite	NiS	+2	-2	Trigonal	R3m
Gersdorffite-Pa3	$Ni(As,S)_2$	2	-2	cubic	
Ullmannite	NiSbS			cubic	$P2_13$
Heazlewoodite	Ni_3S_2			trigonal	R32
Polydymite	Ni_3S_4	+2,+3	-2	cubic	
Vaesite	NiS_2	+2	-1	cubic	Pa3
Parkerite	$Ni_3(Bi,Pb)_2S_2$			monoclinic	
Vysotskite	(Pd,Ni)S	+2	-2	Tetragonal	

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.



Mineral Name	Chemical Composition	Valence State		Crystal Symmetry	
		Co	S	Crystal System	Space Group
Cobaltite	CoAsS	+3		Orthorhombic	$Pca2_1$
Linnaeite	Co_3S_4	+2,+3	-2	Cubic	
Cobaltpentlandite	Co_9S_8			Cubic	Fm3m
Alloclasite	CoAsS			Monoclinic	$P2_1$
Cattierite	CoS_2	+2	-1	Cubic	Pa3
Willyamite	CoSbS	+3		Cubic	
Costibite				Orthorhombic	$Pmn2_1$
Paracostibite				Orthorhombic	
Jaipurite	CoS	+2	-2	Hexagonal	
Julienite	$Na_2Co(SCN)_4.8H_2O$	+2	-2	Monoclinic	$P2_1/n$

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

Fe, Cu							
Mineral Name	**Locality Counts**	**Chemical Composition**	**Valence State**			**Crystal Symmetry**	
			Cu	**Fe**	**S**	**Crystal System**	**Space Group**
Chalcopyrite	26279	$CuFeS_2$	+1	+3	-2	Tetragonal	I42d
Bornite	5293	Cu_5FeS_4	+1	+3	-2	Orthorhombic	Pbca
Cubanite	748	$CuFe_2S_3$	+1	+2,+3	-2	Orthorhombic	2/m2/m2/m
Stannite	632	$Cu_2FeSn_4S_4$	+1	+2	-2	Tetragonal	I42m
Freibergite	630	$Ag_6Cu_4Fe_2Sb_4S_{12}$	+1	+2	-2	Tetragonal	I43m

Valleriite	229	$2[(Fe,Cu)S]\cdot 1.53[(Mg,Al)(OH)_2]$	+2	+2	-2	Hexagonal	
Isocubanite	184	$CuFe_2S_3$	+1	+2,+3	-2	Cubic	Fm3m
Idaite	133	Cu_3FeS_4	+2	+2	-2	Hexagonal	

Fe, Ni							
Mineral Name	**Locality Counts**	**Chemical Composition**	**Valence State**			**Crystal Symmetry**	
			Fe	**Ni**	**S**	**Crystal System**	**Space Group**
Pentlandite	1392	$(Ni,Fe)_9S_8$				Cubic	Fm3m
Mackinawite	424	$(Fe,Ni)_{1+x}S$ (x = 0-0.07)	+2	+2	-2	Tetragonal	P4/nmm
Violarite	361	$FeNi_2S_4$	+2	+3	-2	Cubic	
Smythite	71	$(Fe,Ni)_{3+x}S_4$ (x ≈ 0-0.3)				Trigonal	$R\bar{3}m$
Argentopentlandite	63	$Ag(Fe,Ni)_8S_8$				Cubic	Fm3m
Godlevskite	32	$(Ni,Fe)_9S_8$				Orthorhombic	C222

Table S2 Sulfide minerals with ternary metal compositions.

Mineral Name	**Locality Counts**	**Chemical Composition**
Djerfisherite	57	$K_6(Fe,Cu,Ni)_{25}S_{26}Cl$
Sugakiite	3	$Cu(Fe,Ni)_8S_8$
Kharaelakhite	2	$(Cu,Pt,Pb,Fe,Ni)_9S_8$
Owensite	2	$(Ba,Pb^{2+})_6(Cu^{1+},Fe^{2+},Ni^{2+})_{25}S^{2-}{}_{27}$
Samaniite	2	$Cu_2Fe_5Ni_2S_8$
Ferhodsite	1	$(Fe,Rh,Ni,Ir,Cu,Pt)_9S_8$
Zoharite	1	$(Ba,K)_6(Fe,Cu,Ni)_{25}S_{27}$
Tarkianite	6	$(Cu,Fe)(Re,Mo)_4S_8$
Maikainite	2	$Cu^{1+}{}_{10}Fe^{2+}{}_3Mo^{4+}Ge^{4+}{}_3S^{2-}{}_{16}$
Ovamboite	1	$Cu^{1+}{}_{10}Fe^{2+}{}_3W^{4+}Ge^{4+}{}_3S^{2-}{}_{16}$

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

Mineral Name	Chemical Composition
Delvauxite	$CaFe^{3+}_4(P^{5+}O_4)_2(OH)_8$. 4-5$H_2O$
Diadochite	$Fe^{3+}_2(PO_4)(SO_4)(OH)$. 6$H_2O$
Ekanite	$Ca_2ThSi_8O_{20}$
Evansite	$Al_3PO_4(OH)_6$. 8H_2O
Georgeite	$Cu^{2+}_2CO_3(OH)_2$
Ice	H_2O
Jordisite	$Mo^{4+}S^{2-}_2$
Zaratite	$Ni^{2+}_3C^{4+}O_3(OH)_4$. 4H_2O