

Supplementary Information for

**“Earth’s Volatile Depletion Trend is Consistent with
a High-Energy Moon-Forming Impact”**

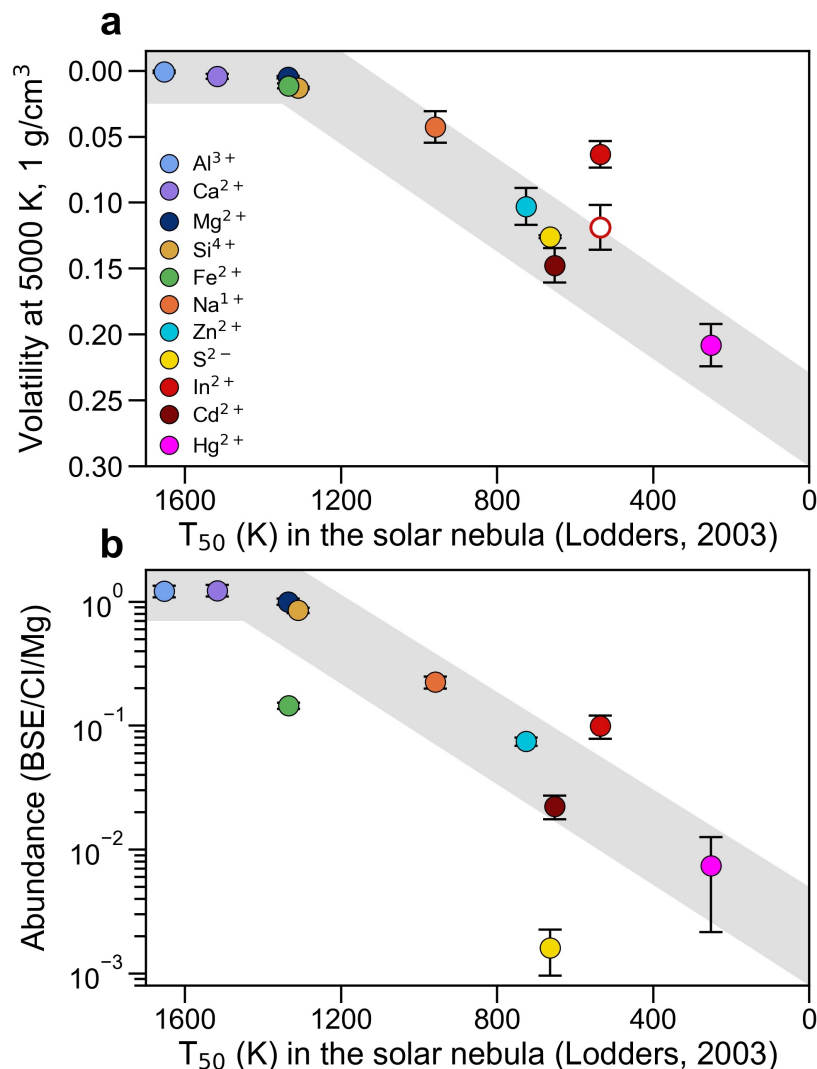
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Supplementary Figures



Supplementary Fig. 1 | Volatile depletion trends using the 50% condensation temperatures (T₅₀) in the solar nebula gas calculated by Lodders¹. The overall trend and deviations are very similar to those in Fig. 2 where the reappraised 50% condensation temperatures of Wood et al.² were used. The calculated volatility of In²⁺ is shown in the absence of S²⁻ (red filled circle) and in the presence of S²⁻ (red open circle). Uncertainties on computed volatilities correspond to the convergence window of the volatilities with simulation time.

Supplementary Tables

Supplementary Table 1. Composition of the volatile-bearing pyrolite melts. Abundances are reported as oxide weight percentages. Here we report the compositions of all the volatile-bearing pyrolite melts considered in this study: (a) In¹⁺-bearing pyrolite melt, (b) In¹⁺-bearing pyrolite melt in the presence of S²⁻, (c) In²⁺-bearing pyrolite melt, (d) In²⁺-bearing pyrolite melt in the presence of S²⁻, (e) In³⁺-bearing pyrolite melt, (f) In³⁺-bearing pyrolite melt in the presence of S²⁻, (g) In³⁺-bearing pyrolite melt in the presence of S⁶⁺, (h) Cd²⁺-bearing pyrolite melt, (i) Zn²⁺-bearing pyrolite melt, and (j) Hg²⁺-bearing pyrolite melt. See Supplementary Table 2 for the stoichiometries.

	a	b	c	d	e	f	g	h	i	j
SiO₂	41.9	41.2	41.1	40.0	42.3	41.1	37.8	41.2	42.9	38.3
MgO	34.0	33.4	31.0	30.2	35.5	34.5	31.7	31.1	32.4	28.9
CaO	3.3	3.2	3.2	3.1	3.3	3.2	2.9	3.2	3.3	3.0
Na₂O	0.9	0.9	0.9	0.9	0.9	0.9	0.8	0.9	0.9	0.8
Al₂O₃	4.4	4.4	4.4	4.2	1.5	1.5	1.3	4.4	4.6	4.1
FeO	8.4	2.1	8.2	2.0	8.4	2.0	7.5	8.2	8.6	7.6
FeS	-	7.5	-	7.3	-	7.5	-	-	-	-
InO	-	-	11.2	-	-	-	-	-	-	-
In₂O	7.1	-	-	-	-	-	-	-	-	-
In₂O₃	-	-	-	-	8.1	-	7.3	-	-	-
InS	-	-	-	12.2	-	-	-	-	-	-
In₂S	-	7.5	-	-	-	-	-	-	-	-
In₂S₃	-	-	-	-	-	9.3	-	-	-	-
CaSO₄	-	-	-	-	-	-	10.7	-	-	-
CdO	-	-	-	-	-	-	-	11.0	-	-
ZnO	-	-	-	-	-	-	-	-	7.3	-
HgO	-	-	-	-	-	-	-	-	-	17.3

Note: The distribution of S²⁻ between InS and FeS (or any other species) is arbitrary, as the pyrolite melt is not physically synthesized from these oxides. We added a sufficient amount of S²⁻ to the system to observe its effect on the vaporization behavior of In.

Supplementary Table 2. Stoichiometry of the volatile-bearing pyrolite melts. Labels (a-j) correspond to the same labeling scheme as in Supplementary Table 1.

a	$\text{NaCa}_2\text{Fe}_4\text{Mg}_{29}\text{Al}_3\text{In}_2\text{Si}_{24}\text{O}_{89}$
b	$\text{NaCa}_2\text{Fe}_4\text{Mg}_{29}\text{Al}_3\text{In}_2\text{Si}_{24}\text{S}_4\text{O}_{85}$
c	$\text{NaCa}_2\text{Fe}_4\text{Mg}_{27}\text{Al}_3\text{In}_3\text{Si}_{24}\text{O}_{89}$
d	$\text{NaCa}_2\text{Fe}_4\text{Mg}_{29}\text{Al}_3\text{In}_3\text{Si}_{24}\text{S}_6\text{O}_{83}$
e	$\text{NaCa}_2\text{Fe}_4\text{Mg}_{30}\text{AlIn}_2\text{Si}_{24}\text{O}_{89}$
f	$\text{NaCa}_2\text{Fe}_4\text{Mg}_{30}\text{Al}_1\text{In}_2\text{Si}_{24}\text{S}_6\text{O}_{83}$
g	$\text{NaCa}_5\text{Fe}_4\text{Mg}_{30}\text{Al}_1\text{In}_2\text{Si}_{24}\text{S}_3\text{O}_{101}$
h	$\text{NaCa}_2\text{Fe}_4\text{Mg}_{27}\text{Al}_3\text{Cd}_3\text{Si}_{24}\text{O}_{89}$
i	$\text{NaCa}_2\text{Fe}_4\text{Mg}_{27}\text{Al}_3\text{Zn}_3\text{Si}_{24}\text{O}_{89}$
j	$\text{NaCa}_2\text{Fe}_4\text{Mg}_{27}\text{Al}_3\text{Hg}_3\text{Si}_{24}\text{O}_{89}$

Supplementary Table 3. A comparison of the 50% condensation temperatures. Here we report the 50% condensation temperatures, as calculated by Lodders¹ and Wood et al.² and the corresponding phases that were used for the calculations of the condensation temperatures. Forsterite, enstatite and clinopyroxene are abbreviated as fo, en, and cpx, respectively.

	Wood et al. (2019)		Lodders (2003)	
	T ₅₀ (K)	Phase	T ₅₀ (K)	Phase
Al	1652	corundum	1653	hibonite
Ca	1535	melilite	1517	hibonite + melilite
Mg	1343	fo + cpx	1336	fo
Si	1314	fo + cpx	1310	fo + en
Fe	1338	Fe alloy	1334	Fe alloy
Na	1035	plagioclase	958	feldspar
Zn	704	FeS	726	fo + n
S	672	FeS	664	FeS
In	492	FeS	536	FeS
Cd	502	FeS	652	en + FeS
Hg	240	FeS	252	FeS

Supplementary Table 4. Proportion of the element existing in the vapor phase at 5000 K and 1 g/cm³. Oxidation states refer to the state in which the elements were added to the melt. The electronic structures are not constrained during the simulation and evolve over time as the local environment changes. Volatility values for In³⁺ and Cd²⁺ were extrapolated from the fitted volatilities, as shown in Figure 1 and error values were determined from the simulation at the closest density. Error values indicate the error on the percent volatility (e.g., the volatility of Na¹⁺ is 4.2% +/- 0.9%) and correspond to the convergence window of the simulations.

Element	Volatility	Error	Element	Volatility	Error
Al ³⁺	0.1%	0.1%	In ¹⁺	4.5%	1.2%
Ca ²⁺	0.4%	0.2%	In ²⁺	6.3%	1.0%
Mg ²⁺	0.5%	0.1%	In ³⁺	3.5%	0.6%
Si ⁴⁺	1.3%	0.1%	In ¹⁺ w/S ²⁻	6.6%	1.3%
Fe ²⁺	1.1%	0.2%	In ²⁺ w/S ²⁻	11.9%	1.7%
Na ¹⁺	4.2%	0.9%	In ³⁺ w/S ²⁻	6.6%	0.4%
Zn ²⁺	10.3%	1.4%	In ³⁺ w/S ⁶⁺	4.3%	0.5%
Cd ²⁺	14.8%	1.4%	S ²⁻ w/In ³⁺	12.6%	0.2%
Hg ²⁺	20.8%	1.6%	S ⁶⁺ w/In ³⁺	29.2%	1.6%

Supplementary Table 5. Types of vaporized species containing each volatile element at ~1 g/cm³ and 5000 K. For the In³⁺-bearing system, abundances are averaged over densities of 0.97 and 1.06 g/cm³. Due to the low abundance of Al and Ca in the pyrolite system and their refractory nature (remaining almost entirely in the melt phase at 5000 K), their speciation in the vapor is not possible to accurately evaluate.

Mg ²⁺	Mg (35%), MgO (17%), MgSiO ₂ (15%), MgSiO ₃ (6%), MgSi ₂ O ₅ (3%), MgO ₂ (2%), MgSiO ₄ (2%), MgSi ₃ O ₅ (2%), MgInSi ₂ O ₆ (2%), Mg ₂ FeSiO ₆ (2%), Mg ₂ Si ₂ O ₆ (2%)
Si ⁴⁺	SiO (42%), SiO ₂ (26%), MgSiO ₂ (9%), SiO ₃ (4%), MgSiO ₃ (3%), CaSiO ₂ (2%), MgSi ₂ O ₅ (2%), MgSiO ₄ (1%), MgSi ₃ O ₅ (1%), MgSi ₂ InO ₆ (1%), FeMg ₂ SiO ₆ (1%), Mg ₂ Si ₂ O ₆ (1%), Mg ₂ Si ₃ O ₅ (1%)
Fe ²⁺	FeO (34%), FeO ₂ (22%), FeO ₃ (17%), FeMgO ₃ (5%), FeMg ₂ SiO ₆ (5%), FeMgO ₂ (4%), FeSiO ₂ (3%), FeSiO ₄ (3%), FeMgSi ₂ O ₆ (2%), FeMgSiO ₅ (2%), Fe (1%), FeMg ₂ AlO ₃ (1%)
Na ¹⁺	Na (76%), NaO ₂ (18%), NaSiO ₃ (1%), NaO (1%)
Zn ²⁺	Zn (93%), SiZnO ₂ (2%), SiZnO ₃ (2%), ZnO ₂ (2%), ZnO (1%)
Cd ²⁺	Cd (90%), CdO (4%), CdO ₂ (1%), SiCdO ₂ (1%)
Hg ²⁺	Hg (87%), SiHgO ₂ (3%), HgO (3%), FeSiHgO ₃ (2%), HgO ₂ (1%)
In ¹⁺	In (76%), InSiO ₂ (9%), InO (7%), InSiO ₃ (4%), InSi ₂ O ₄ (2%), InMgSi ₂ O ₅ (2%)
In ²⁺	In (79%), InO (6%), InSiO ₂ (5%), InSiO (3%), InO ₂ (2%), InMgSiO ₄ (2%), InFeO ₂ (2%)
In ³⁺	In (69%), InO ₂ (13%), InO (8%), InO ₃ (4%), InMgSi ₂ O ₆ (4%), InSiO (1%)
In ¹⁺ w/S ²⁻	In (84%), InSiO ₂ (6%), InO (3%), InSiO (1%), InO ₂ S (1%), InMgSiO ₂ (1%), InOS (1%)
In ²⁺ w/S ²⁻	In (59%), In ₂ O (7%), InO ₂ S (7%), InFeSiO ₃ (6%), InSiO (5%), InO (4%), InMgSiO ₄ (3%), InO ₃ S (2%), InAlSiO ₃ (2%), InFeSi ₂ O ₄ (2%), InSiS (2%)
In ³⁺ w/S ²⁻	In (59%), InO (7%), InSiO ₂ (7%), InSiO (5%), InOS (4%), InO ₂ S (3%), FeInO (3%)
In ³⁺ w/S ⁶⁺	In (77%), InO (8%), MgInO ₃ (3%), MgInO ₂ (2%), InSiO ₃ (2%) and InSiO ₄ (2%)
S ²⁻ w/ In ³⁺	SO ₂ (41%), SO (34%), S (7%), S ₂ (2%), InOS (1%), MgSiOS (1%), MgO ₂ S (1%), MgOS (1%), InO ₂ S (1%)
S ⁶⁺ w/ In ³⁺	SO ₂ (39%), SO (29%), S (28%), SO ₃ (1%)

Supplementary Notes

Supplementary Note 1

Indium exists in a range of oxidation states. With the presence of the highly reduced solar nebula gas, In likely existed in the +2 oxidation state². The 50% condensation temperature for In has thus only been calculated for In²⁺ into InS, as it was likely the dominant In-bearing phase in the solar nebula gas during Earth's accretion^{1,2}. However, In²⁺ is likely not a representative oxidation state after the Moon-forming impact, as the nebular gas would have dissipated within the first 3 million years³ of the global magma ocean that existed after the Moon-forming impact was established by silicate-gas equilibria under much more oxidizing conditions compared to the solar nebula gas. In the present-day Earth, In exists almost exclusively in the +3 oxidation state, as seen in sulfide and oxide minerals, such as sphalerite^{4,5}, cassiterite^{6,7}, chalcopyrite^{4,8} and stannite⁶. Furthermore, mineral-melt partitioning experiments have shown that In is incorporated into biotite and amphibole in the +3 oxidation state⁹, strongly suggesting that In would have existed as In³⁺ in the early magma ocean. There have also been some studies exploring the +1 oxidation state^{2,10,11}. In the melt-silicate partitioning experiments of Wang et al.¹², In was added as In₂O (+1 oxidation state) while in dissolution experiments on molten CaO-SiO₂-Al₂O₃ slags at highly reducing conditions, In was found to exist with the -1 and +1 oxidation states for silica contents of <20 wt% and >20 wt%, respectively^{10,11}. However, it is unclear under what geological conditions In would exist in the -1 and +1 oxidation states.

Here, we compute the vaporization behavior of In added to pyrolite melt in the +3 oxidation state through substitution for Al³⁺ at densities of ~0.95 to 2.6 g/cm³ and temperatures of 4000 K, 5000 K and 6000 K. To compare our results to previous studies, we also calculate the vaporization behavior of In added to pyrolite melt in the +1 and +2 oxidation states at 1 g/cm³

and 5000 K. Our results indicate that In^{2+} is more volatile than In^{3+} , which may explain the apparent overabundance of In in the Earth relative to CI chondrites (see main text).

S is also found in various oxidation states, ranging from -2 and +6. Generally, S exists in the -2 oxidation state at $\log f\text{O}_2 < \text{FMQ}-1$, in the +6 oxidation state at $\log f\text{O}_2 < \text{FMQ}+2$ and in a multiple oxidation states at intermediate oxygen fugacity conditions¹³⁻¹⁵. The 50% condensation temperature for S has been calculated for the -2 oxidation state into FeS due to the reducing nature of the solar nebula gas. In this study, we consider the endmember oxidation states, S^{2-} and S^{6+} . We examine the effect of S^{2-} on the vaporization behavior of In^{1+} , In^{2+} and In^{3+} and the effect of S^{6+} on the vaporization behavior of In^{3+} at 5000 K and 1 g/cm³. Although In and S are added to the system with a set oxidation state (e.g., In_2O , InO or In_2O_3), the electronic structures are not constrained throughout the simulation and evolve with time, depending on the local chemical environment.

Supplementary Note 2

The base pyrolite melt in our study is a six-component melt with a molar composition of $0.5\text{Na}_2\text{O} - 2\text{CaO} - 1.5\text{Al}_2\text{O}_3 - 4\text{FeO} - 30\text{MgO} - 24\text{SiO}_2$ where the six components are within 1 wt% of the nominal bulk silicate Earth composition¹⁶. The elemental concentration of In and Cd in the bulk silicate Earth are estimated as 11 and 40 ppb, respectively¹⁶. In this study we examine the partitioning behavior of trace elements between pyrolite melt and vapor. Due to computational feasibility, the pyrolite melts in our study contain 7 wt% In^{3+} and 10 wt% Cd^{2+} (melts “e” and “h” in Supplementary Tables 1 and 2), respectively. We have previously explored the effect of concentration on the partitioning behavior of volatile elements in pyrolite melt and did not observe a difference in vaporization behavior for the range of concentrations explored¹⁷.

Ab initio molecular dynamics simulations are typically limited to 100-200 atoms due to the cubic-scaling cost associated with methods based on density functional theory. In these types of simulations, it is important to acquire sufficient statistics (i.e., to achieve convergence over time) in order to report meaningful vaporization proportions. Increasing the occurrence of the event of interest (i.e., the vaporization of the element) increases the statistical quality and decreases the error associated with the calculated vaporization proportion. This can be accomplished via longer simulation times and/or a larger concentration of the element of interest. Our low-density simulations (at 1 g/cm³) with ~150-170 atoms produce about 200 time steps per day, parallelized on high-performance supercomputers. To achieve 20 ps, it thus takes 100 days of uninterrupted simulation time. To achieve 20 ps with a trace-element concentration that is even 1/2 or 1/4 of the present concentration, we would increase the number of atoms in our simulation 2-fold and 4-fold, which would result in a 8-fold and 64-fold increase in the required computational time, respectively.

With future advancements in machine-learning potentials based on *ab initio* molecular dynamics, it may become feasible to compute the vaporization behavior of trace elements in more realistic concentrations. Until then, the present study is a rigorous method based on first principles to calculate the melt-vapor partitioning behavior of elements with the available computational resources and technologies. The calculations performed in this study are novel and important for our understanding of the behavior of trace elements in silicate melts, and the results agree remarkably well with the experiments of Norris and Wood¹⁸ on the volatility of In and Zn, providing a novel avenue for study of trace element volatility at Early Earth conditions.

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