Carbon as the dominant light element in the lunar core

Edgar S. Steenstra¹, Yanhao Lin¹, Nachiketa Rai²,³, Max Jansen¹, Wim van Westrenen¹

¹Faculty of Earth and Life Sciences, Vrije Universiteit, Amsterdam, The Netherlands
²Centre for Planetary Sciences, Birkbeck–UCL, London, United Kingdom
³Department of Earth Sciences, Mineral and Planetary Sciences Division, Natural History Museum, London, United Kingdom

ABSTRACT

Geophysical and geochemical observations point to the presence of a light element in the lunar core, but the exact abundance and type of light element are poorly constrained. Accurate constraints on lunar core composition are vital for models of lunar core dynamo onset and demise, core formation conditions (e.g., depth of the lunar magma ocean or LMO) and therefore formation conditions, as well as the volatile inventory of the Moon. A wide range of previous studies considered S as the dominant light element in the lunar core. Here, we present new constraints on the composition of the lunar core, using mass balance calculations, combined with previously published models that predict the metal–silicate partitioning behavior of C, S, Ni and recently proposed new bulk silicate Moon (BSM) abundances of S and C. We also use the bulk Moon abundance of C and S to assess the extent of their devolatilization. We observe that the Ni content of the lunar core becomes unrealistically high if shallow (<3 GPa) LMO scenarios are assumed, and therefore only deeper (>3 GPa) LMO scenarios are considered for S and C. The moderately siderophile metal–silicate partitioning behavior of S during lunar core formation, combined with the low BSM abundance of S, yields only <0.16 wt% S in the core, virtually independent of the pressure (P) and temperature (T) conditions during core formation. Instead, our analysis suggests that C is the dominant light element in the lunar core. The siderophile behavior of C during lunar core formation
results in a core C content of ~0.6–4.8 wt%, with the exact amount depending on the core formation conditions. A C–rich lunar core could explain (1) the existence of a present–day molten outer core, (2) the estimated density of the lunar outer core and (3) the existence of an early lunar core dynamo driven by compositional buoyancy due to core crystallization. Finally, our calculations suggest the C content of the bulk Moon is close to its estimated abundance in the bulk silicate Earth (BSE), suggesting more limited volatile loss during the Moon-forming event than previously thought.

**Keywords:** Moon, Lunar, Core, Siderophile, Volatiles

**INTRODUCTION**

Geophysical and geochemical observations suggest the lunar core contains several wt% of one or more light elements. One constraint on the abundance and nature of the light element inventory stems from a reanalysis of Apollo era lunar seismograms suggesting the existence of a partially molten outer core (Weber et al. 2011), which requires the presence of one or more light elements to reduce the liquidus of the core. The existence of an ancient lunar core dynamo (e.g., Cisowski et al. 1983; Collinson 1993; Shea et al. al. 2012) suggests the presence of one or more light elements in the lunar core, which is required to drive compositional convection in the lunar core (e.g., Laneuville et al. 2014). Light elements H, O and Si are not expected to significantly partition into the lunar core because the oxygen fugacity during lunar core formation was either too oxidizing (Si), or because the pressure in the Moon (~5 GPa at the core-mantle boundary, ~5.3 GPa in the center; Garcia et al. 2011, 2012) is too low (Killburn and Wood 1997; Ricolleau et al. 2011; Steenstra et al. 2016b).

From molten metal alloy density and liquidus considerations, Weber et al. (2011) proposed that the lunar core contains less than 6 wt% of lighter alloying elements. Sulfur (S) was deemed the most likely candidate, because of its high solubility in Fe metal, and its ability to
significantly reduce the bulk density, sound velocity and liquidus temperature of the lunar core (e.g., Hauck et al. 2006; Weber et al. 2011; Jing et al. 2014). Follow-up studies therefore primarily focused on assessing the feasibility of S in the lunar core. For example, Laneuville et al. (2013) suggested from thermochemical evolution models that ~3 wt% S would be required for the crystallization of a 240 km radius lunar inner core, whereas Zhang et al. (2013) propose lunar core S contents of ~5–10 wt%. Laneuville et al. (2014) proposed from thermochemical modeling of the lunar core dynamo an initial S core content of 7±1 wt%, or alternatively, more than 12 wt% if the Moon never crystallized an inner core. From Fe–S equation of state measurements, Jing et al. (2014) prefer a lunar core model with 4±3 wt% S, whereas Antonangeli et al. (2015) propose S core contents of 8.5±2.5 wt%, based on compressional and shear wave sound velocity and density measurements of γ–Fe at high pressures and temperatures. Rai and van Westrenen (2014) showed that the lunar mantle depletions of Cr and V can be explained by metal–silicate segregation of a lunar core containing 6 wt% S, if temperatures during core formation are limited to the lunar mantle liquidus. Steenstra et al. (2016b) showed that the depletions of 15 siderophile elements (including V and Cr) in the lunar mantle can also be explained at much lower S contents if super–liquidus temperatures during core formation are considered.

It is as of yet unclear how these proposed S contents of the lunar core relate to the lunar mantle or bulk silicate Moon (BSM) abundance of S. If single stage equilibrium between the lunar core and mantle occurred, which seems likely given the siderophile element depletion pattern in the lunar mantle (Rai and van Westrenen, 2014; Steenstra et al., 2016b), the proposed abundance of S in the lunar core must be compatible, at least to a reasonable extent, with the amount of S in the BSM.

From its siderophile behavior (Dasgupta et al. 2013; Chi et al. 2014) and its ability to significantly decrease both the Fe–metal liquidus and density relative to pure Fe (e.g., Chabot...
et al. 2008; Sanloup et al. 2011) carbon (C) is another light element that could be present in the lunar core. However, the role of C was not quantitatively considered previously. Using recently proposed BSM abundances of C and S in conjunction with recently published models that describe their metal–silicate partitioning behavior as a function of pressure ($P$), temperature ($T$), composition of the silicate and metal (X) and oxygen fugacity ($fO_2$), here we re-assess the likelihood of one or both of these light elements are present in significant amounts in the lunar core. We also use these results to compare the lunar S and C inventories with their abundances in the bulk silicate Earth (BSE) to assess volatile loss from the Moon.

**METHODS**

We adopt a simple mass balance approach (e.g., Righter 2002) with which the amount of element $i$ in the lunar core or mantle can be calculated (Eqs. 1, 2):

$$C_{\text{core}}^i = \frac{C_{\text{BM}}^i}{x_{\text{core}} + (1 - x_{\text{core}})/D(i)}$$  \hspace{1cm} (1)

$$C_{\text{mantle}}^i = \frac{C_{\text{BM}}^i}{x_{\text{mantle}} + (1 - x_{\text{mantle}}) * D(i)}$$  \hspace{1cm} (2)

in which $C^i$ is defined as concentration of element $i$ in the lunar core, $C_{\text{BM}}^i$ as the concentration by weight of element $i$ in the bulk Moon (BM), $x$ is either the core or lunar mantle mass fraction and $D(i)$ is the metal–silicate partition coefficient $D$ for element $i$. We calculate $D($Ni, S, C$)$ for three core formation scenarios detailed below (Table 1) by using the predictive models proposed by Rai and van Westrenen (2014), Boujibar et al. (2014) and Chi et al. (2014) for Ni, S and C, respectively. For each scenario, we calculate the amount of S and C at these $P$-$T$ conditions and corresponding Ni contents.
Scenario 1 assumes a metal-silicate equilibration pressure during core formation of 3 GPa, corresponding to the presence during core formation of a lunar magma ocean with a depth of ~650 km. This depth corresponds to the depth from which deep moonquakes occur (>700 km, Nakamura et al., 1973), which could reflect the minimum original depth of the lunar magma ocean (Elkins-Tanton et al., 2011).

The maximum metal-silicate equilibration pressure of 4.8 GPa used in scenarios 2 and 3 is constrained by the estimated pressure at the core-mantle boundary (Garcia et al., 2011, 2012). These two scenarios therefore assume whole-Moon melting at the time of core formation. This seems plausible given the estimated disk midplane temperature (>3000-7000 K) derived from giant impact based lunar formation models (e.g., Canup, 2004; Nakajima and Stevenson, 2014; Hauri et al., 2015). Metal-silicate equilibration temperatures in whole-Moon melting models can range between the liquidus and the disk midplane temperature. Studies that linked the lunar mantle siderophile element depletions to their experimentally determined metal-silicate partitioning behavior also found that the Moon likely formed hot. Rai and van Westrenen (2014) found that the lunar mantle siderophile element depletions of Ni, Co, W, Mo, P, V, and Cr can be reconciled with formation of a <6 wt% S-bearing core in a fully molten Moon at liquidus temperatures. For scenarios 1 and 2, we therefore use the temperature ranges that are constrained by the lunar mantle liquidus parameterization proposed by Suckale et al. (2011) (Table 1). A follow up study of Steenstra et al. (2016b) extended this work and found that a lunar core with several wt% S is not required for the lunar mantle depletions of 15 siderophile elements if the lunar core formed at super-liquidus conditions in a fully molten Moon (T ~ 3150 ± 200 K). In scenario 3, we use the latter super-liquidus temperature range (Table 1).

The oxygen fugacity ($fO_2$) relative to the iron–wüstite buffer ($\Delta IW$) is constrained to $\Delta IW = –2$, a reasonable estimate given the FeO content of the lunar mantle (e.g., Rai and van
Westrenen 2014 and references therein). To quantify the possible silicate melt compositional effects on $D(C, S, Ni)$, we consider an average of many recently proposed BSM compositions and corresponding $nbo/t$ ratio of 2.55 in all three scenarios (Rai and van Westrenen, 2014) and references therein). Boujibar et al. (2014) and Chi et al. (2014) showed that the metal–silicate partitioning of $S$ and $C$ is dependent on the Ni content of the metal. We take this effect into account by calculating the predicted Ni content of the lunar core following each scenario, and using these Ni contents to calculate $D(C, S)$ (Table 1). We therefore model either a Fe–Ni–S ($X_C^{met} = 0$) alloy or Fe–Ni–C ($X_S^{met} = 0$) alloy. We assume that no Si or O is dissolved in the lunar core ($X_{Si}^{met}$ and $X_O^{met} = 0$). For $C$, our approach is validated by the negligible effect of up to 5 wt% $S$ on $D(C)$ (Li et al. 2015). However, $D(S)$ has been shown to decrease with increasing $C$ in the metal liquid (Boujibar et al. 2014). This would decrease $D(S)$ if a $C$–rich lunar core would be considered. We will later show that the abundance of $S$ in the lunar core is already very limited for a lunar core with $X_C^{met} = 0$, so we conclude that this effect will not change the outcome of our study.

The required BM abundances of $C$, $S$, and Ni are calculated with the derived metal–silicate partition coefficients ($D$’s) and are combined with Eq. (3):

$$D_{mantle}^{core}(i) = \frac{C_{BM}^i - x_{mantle} \cdot C_{BSM}^i}{C_{BSM}^i} \left[ C_{BSM}^i \cdot (1 - x_{mantle}) \right]$$  \hspace{1cm} (3)

Rearranging yields Eq. (4):

$$C_{BM}^i = D_{mantle}^{core}(i) \cdot C_{BSM}^i \cdot (1 - x_{mantle}) + x_{mantle} \cdot C_{BSM}^i$$  \hspace{1cm} (4)

where $D_{mantle}^{core}(i)$ (or $D(i)$) is the required metal–silicate partition coefficient for element $i$, and $C_{BSM}^i$ is the bulk silicate Moon (BSM) abundance of element $i$. The advantage of this
approach is that the outcome is independent of the assumed lunar core mass. We use the BSM estimates of 470±50 ppm for Ni (Delano 1986), 74.5±4.5 ppm for S (Hauri et al. 2015; Chen et al. 2015) and 54±10 ppm for C (Wetzel et al. 2015). Table 1 lists the $P$–$T$ conditions during lunar core formation that we explore in this study, as well as the calculated $X_{Ni}$ content of the lunar core at these conditions, used to calculate $D(C, S)$.

RESULTS

Nickel

Nickel is considered as one of the major alloying elements in planetary cores, because of its high abundance in primitive materials and its strongly siderophile tendencies at the $P$–$T$–$fO_2$ conditions relevant for planetary differentiation. The metal–silicate partitioning behavior of Ni as a function of $P$–$T$–$X$–$fO_2$ at lunar relevant conditions is well quantified (Rai and van Westrenen 2014; Steenstra et al. 2016a, b) and mainly varies as a function of $P$, $T$, and $fO_2$. The $fO_2$ during lunar core formation is well constrained to $\Delta IW = -2$ by the FeO content of the lunar mantle (e.g., Rai and van Westrenen 2014), leaving $P$ and $T$ as the dominant variables affecting $D(Ni)$ (Fig. 1). Due to the strong increase of $D(Ni)$ with decreasing temperature, we obtain unrealistically high Ni contents of the lunar core for shallow LMO scenarios (<3 GPa) when using the Ni content of the lunar mantle of 470±50 ppm (Delano 1986). For example, core–mantle equilibration at 1 GPa would have resulted in an lunar Ni core content of >56 wt%. In the following calculations, we therefore focus on scenarios where the LMO equilibrated with the lunar core at depths greater than ~650 km (corresponding to $P$ >3 GPa). We note that a deep LMO is also suggested from a wide range of other siderophile element depletions in the lunar mantle (Rai and van Westrenen 2014; Steenstra et al. 2016b).
Sulfur

Recent analyses of a wide range of lunar volcanic glasses (Hauri et al. 2015) and various lunar melt inclusions (Chen et al. 2015) suggest that the BSM contains 74.5±4.5 ppm of sulfur. The predictive equation for log D(S) provided by Boujibar et al. (2014) suggests that the metal–silicate partitioning behavior of S at lunar relevant conditions mainly varies as a function of $P$, the FeO content of the lunar mantle and the Ni content of the lunar core (Fig. 1). For each of the three scenarios, we calculate an overall log D(S) range of ~0.25–1.30. Using the BSM estimates of Chen et al. (2015) and Hauri et al. (2015), this corresponds to BM abundances ranging between ~71–116 ppm S, somewhat lower than the estimated bulk silicate Earth (BSE) content of 250±50 ppm S (McDonough and Sun 1995). Using a BM abundance of ~71–116 ppm S, the resulting lunar core S content is only ~0.01–0.16 wt%, with the exact amount depending on the scenario considered (Table 1). An example is given in Fig. 2a, where the estimated lunar core and mantle S content is calculated if scenario 2 is considered. The maximum S core content (~0.14±0.02 wt%) is expected for a deep LMO with super–liquidus temperatures (scenario 3), whereas assuming an intermediate depth LMO (3 GPa, scenario 1) and corresponding liquidus temperatures, would result in even lower S content (0.02±0.01 wt%). An important observation is the minor variation in estimated core S content, across a wider range of log D(S) values (Table 2). We conclude that the calculated lunar core S abundances are close to 2 orders of magnitude lower than those proposed from other studies (e.g., Weber et al. 2011; Jing et al. 2014; Laneuville et al. 2013, 2014; Antonangeli et al. 2015) irrespective of core formation conditions.

Carbon

Recent high–precision measurements of indigenous C contents in primitive lunar volcanic glasses and melt inclusions, combined with solubility and degassing model calculations,
suggest that the BSM contains 54±10 ppm C (Wetzel et al. 2015). The metal–silicate partitioning behavior of C has been shown to be strongly dependent on $P$, $T$, $fO_2$ and silicate melt composition, approximated with parameter $nbo/t$ in this study (Dasgupta et al. 2013; Chi et al. 2014; Li et al. 2015). At the conditions relevant for lunar core formation, this results in relatively siderophile behavior of C, relative to S (Fig. 1). We calculate an overall lunar core C content range of ~0.6–4.8 wt%, with the exact amount dependent of the core formation scenario considered (Table 1). An example of such a calculation is shown in Fig. 2b. The maximum lunar core C content (3.6±1.2 wt%) is expected for scenario 2. For a deep LMO with super–liquidus conditions, the C core content is reduced to ~2.2±0.9 wt% and for an intermediate depth LMO to ~1.1±0.5 wt% (Table 2). We conclude that in all scenarios C has strongly siderophile behavior, resulting in C being a feasible candidate for the light element in the lunar core. We calculate a range of ~740±520 ppm C in the bulk Moon. This range is in perfect agreement with the estimated C content of the BSE of ~765±300 ppm C (Marty 2012), emphasizing the similarity between the BM and BSE (e.g., de Meijer et al. 2013) and the apparent minor extent of devolatilization depletion of the Moon relative to BSE.

DISCUSSION

Uncertainty in bulk silicate Moon estimates

One potential source of error in our models is uncertainty in the assumed BSM abundances of S and C. For example, the concentration of S and C in lunar rocks could have been affected by devolatilization processes on the Moon after lunar core formation. One way to assess the loss of S following core formation is to study the S isotope compositions of lunar basalts. Wing and Farquhar (2015) measured the S isotope compositions for a wider range of lunar mare basalts, including primitive (low–Ti) mare basalts, and suggest only 1–10 % of S was lost due to degassing processes. This range falls largely within the error bars on the BSM
estimate for S that we consider here. Moreover, three independent studies report very similar
S contents of the BSM (Bombardieri et al. 2005; Chen et al. 2015; Hauri et al. 2015) for a
variation of lunar sample types. Another potential issue is the crystallization of sulfides, through
which S (and other siderophile elements, such as C) could be removed from mare basalts prior
to eruption. However, Bombardieri et al. (2005) found no evidence for sulfide saturation of
the mare basalts. Unless the mare basalts experienced significant S loss, which is not recorded
in the S isotope composition of the lunar basalts, sulfide saturation cannot have occurred.

We also note that even if the primitive BSM concentrations of S and C are significantly
underestimated, the general outcome of this study will not change. For example, assuming a
BSM abundance of 300 ppm S, corresponding to the upper estimate for the BSE, would still
result in less than ~0.6 wt% S in the lunar core. On the contrary, assuming a slightly higher
BSM for C drastically increases its abundance in the lunar core. For example, 80 ppm C in the
lunar mantle would result in a lunar core C content of ~1.3–6.0 wt% C, emphasizing the
geochemical feasibility of C as the dominant light element in the lunar core. The overall
conclusion that C should be far more abundant in the lunar core than S is also robust.

Comparison with geophysical observations

The presence of a specific light element in the lunar core should also be compatible with
geophysical observations. Density, sound velocity and physical state of the lunar core may
provide valuable constraints on lunar core composition. Weber et al. (2011) and other recent
studies of the geophysical properties of the lunar outer core suggest $V_p$ values of 4.1±0.2 km/s
(Weber et al. 2011; Jing et al. 2014). Unfortunately, the physical parameters (e.g., Gruneisen
parameter, shear modulus, thermal expansivity) of Fe–C liquids are poorly constrained, which
prohibits a quantitative assessment. However, C is known to lower $V_p$ relative to pure Fe due
to its effect on lowering the density and bulk modulus of Fe–alloys, similar to S. Another
important proxy for the nature of the light element in the lunar outer core is density. The density of the lunar outer core was constrained by Weber et al. (2011) to $\sim$5.1 g/cm$^3$. However, from sound velocity data of Fe–FeS liquids Jing et al. (2014) suggest the lunar outer core is much denser ($\sim$6.5±0.5 g/cm$^3$), whereas Antonangeli et al. (2015) propose a lunar outer core density of $\sim$5.25±1.75 g/cm$^3$ based on compressional and shear wave sound velocity and density measurements of $\gamma$–Fe. These ranges illustrate the major uncertainty in the lunar outer core density. It is noteworthy to mention that the estimated density ranges of liquid Fe + 5.7 wt% C and liquid Fe + 3.5 wt% C at 5 GPa (Sanloup et al. 2011; Shimoyama et al. 2013), based on X–ray absorption techniques, fall within or are close the latter density ranges. We also note that that the density of Fe–C and Fe–S melts, at identical pressure and temperature (4 GPa, 1923 K) do not show significant differences, except for very S rich compositions (Shimoyama et al. 2013), which is ruled out from low BSM abundances of S.

Like S, C also significantly decreases the liquidus temperatures of Fe alloys (e.g., Chabot et al. 2008). For example, the liquidus temperature for the Fe–C eutectic composition is $\sim$1500±25 K at 5 GPa (Chabot et al. 2008) relative to $\sim$2000 K for pure Fe and $\sim$1260±25 K at 6 GPa for Fe–S (Buono and Walker 2011). The presence of C in the lunar core could therefore explain the partially molten state of the lunar outer core (Weber et al. 2011).

Finally, an important constraint on the light element composition of the lunar core is the former existence of a lunar core dynamo. If we assume the lower boundary for the present-day core-mantle boundary temperature of $\sim$1650 K (Weber et al. 2011; Antonangeli et al. 2015), required for the presence of a partial silicate melt layer at the lunar core–mantle boundary, $\gamma$–Fe would crystallize at C contents below $\sim$3.8 wt% and could form the inner core. This could lead to compositional heterogeneity and buoyancy in the outer core, which can help to initiate and sustain an early lunar core dynamo (Chabot et al. 2008). A Fe$_3$C inner core seems unlikely given the solubility limit of C of $\sim$6 wt% in Fe-Ni melts at these
conditions (Chi et al. 2014), as well as from sound velocity measurements of the lunar inner core (Antonangeli et al. 2015). The errors on the geophysical lunar interior structure properties discussed here are substantial, even with the new data obtained from the SELENE (Selenological and Engineering Explorer or Kaguya) and GRAIL (Gravity Recovery and Interior Laboratory) missions (Yamada et al. 2014). Overall, we conclude that from current geophysical constraints, a C-rich lunar core needs to be seriously considered.

**IMPLICATIONS**

This work suggests from geochemical considerations that C should be the dominant light element in the lunar core, given its highly siderophile tendencies and high abundance in the BSM. This results in an estimated C core content range of ~0.6–4.8 wt% for a wider range of core formation scenarios. This demonstrates the geochemical feasibility of a C-rich lunar core, instead of a S-rich lunar core as previously suggested. In addition, given the amount of S in the lunar core we calculate here (<0.16 wt% S across a wider range of core–mantle equilibration scenarios), it would be difficult to maintain a partially molten core over a long temperature/time interval without another or additional light elements. A C–rich core would explain (1) the present day molten lunar outer core, (2) the suggested density deficit of the lunar outer core and possibly (3) the existence of a (partly) compositionally driven core dynamo through crystallization of Fe metal. Our hypothesis of a C-rich lunar core can be tested by (1) additionally constraining the physical properties of Fe–C liquids at lunar relevant conditions, (2) numerically assessing the feasibility of a lunar core dynamo for a C–rich lunar core and (3) assessing if the siderophile element depletions in the lunar mantle can be reconciled with metal–silicate segregation of a C–rich lunar core. Finally, we note that the BM estimates derived in this study for S and C are relatively close to the estimated BSE abundances of these elements, which confirms once again the close compositional similarities.
between the BM and BSE, as well as the lack of significant devolatilization during the Moon–
forming event. This conclusion is consistent with recent observations for other volatile
elements, e.g., H_2O (Hauri et al. 2015) and a wide range of volatile siderophile elements
(Steenstra et al. 2016b).

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REFERENCES CITED

Antonangeli, D., Morard, G., Schmerr, N.C., Komabayashi, T., Krisch, M., Fiquet, G., and
element and primary sulfur concentrations in Apollo 12 mare basalts: The view from melt
Boujibar, A., Andrault, D., Bouhifd, M.A., Bolfan–Casanova, N., Devidal, J.–L., and Trcera,
N. (2014) Metal–silicate partitioning of sulphur, new experimental and thermodynamic


**Figure captions**

**Figure 1.** The modeled partitioning behavior of C, S, and Ni along the $P$ and corresponding solidus–liquidus $T$ range (Suckale et al. 2012) relevant for the lunar interior, assuming $\Delta IW = -2$, $nbo/t = 2.55$, and $X_{Ni} = 0.20$ for D(C, S). D(C, S, Ni) were modeled using predictive equations from Boujibar et al. (2014) for S, Chi et al. (2014) for C, and Rai and van Westrenen (2014) for Ni.

**Figure 2.** The expected abundance of light elements in the lunar core or mantle, as a function of bulk Moon (BM) abundance, assuming $\Delta IW = -2$, $P = 4.8$ GPa, $T = 2250$ K, $nbo/t = 2.55$ and $X_{Ni} = 0.21\pm0.02$, calculated using Eqs. (1–4) and the predictive models for D(S) of Boujibar et al. (2014) and D(C) of Chi et al. (2014). Panel (a) shows the results for S, with the horizontal lines representing the BSM estimates from Bombardieri et al. (2005), Chen et al. (2015) and Hauri et al. (2015) and vertical lines the range of corresponding BM abundances. Panel (b) shows the estimated lunar core and mantle content for C, with the horizontal lines representing the BSM estimate from Wetzel et al. (2015) and vertical lines the lower and upper limit of the BM abundance. Also displayed is the estimated carbon solubility limit in Fe–rich melts derived from Chi et al. (2014).
Table 1 Modeled $P$–$T$ conditions with corresponding log $D$(Ni, S, C), resulting mole fraction of Ni in the lunar core, and estimated abundances (ppm or wt%) of carbon and sulfur in the lunar core, assuming $fO_2$ of $\Delta IW = –2$ and $nbo/t = 2.55$

<table>
<thead>
<tr>
<th>Scenario</th>
<th>P (GPa)</th>
<th>T (K)</th>
<th>Nickel (Ni)</th>
<th>Sulfur (S)</th>
<th>Carbon (C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1) Intermediate LMO</td>
<td>3.0</td>
<td>2150</td>
<td>2.88</td>
<td>0.34±0.04</td>
<td>0.46±0.21</td>
</tr>
<tr>
<td>2) Deep LMO [1]</td>
<td>4.8</td>
<td>2250</td>
<td>2.67</td>
<td>0.21±0.02</td>
<td>1.17±0.08</td>
</tr>
<tr>
<td>3) Deep LMO [2]</td>
<td>4.8</td>
<td>3150±200</td>
<td>2.45±0.04</td>
<td>0.13±0.03</td>
<td>1.26±0.03</td>
</tr>
</tbody>
</table>

Figure 2a

- **Core**
- **Mantle**
- **BSM 74.5±4.5 ppm**

**Equations and Conditions:**
- $\Delta IW = -2$
- $P = 4.8 \text{ GPa}$
- $T = 2248 \text{ K}$
- $nbo/t = 2.55$
- $X_{Ni} = 0.21\pm0.02$
Estimated solubility limit in Fe-Ni systems

(b)

C in Lunar Mantle or Core (ppm)

Core
BSM 54±10 ppm
BM 951±303 ppm

Mantle

C in bulk Moon (ppm)

ΔIW = -2
P = 4.8 GPa
T = 2248 K
nbo/t = 2.55
X$_{Ni}$ = 0.21±0.02

Figure 2b