

1 **Title**

2 Core Formation and Geophysical Properties of Mars

3 **Authors**

4 Matthew C. Brennan*¹, Rebecca A. Fischer¹, Jessica C. E. Irving²

5 ¹Harvard University, Department of Earth and Planetary Sciences

6 ²Princeton University, Department of Geosciences

7 *Corresponding author contact: 20 Oxford St, Cambridge MA 02138.

8 (617) 998-1514

9 mcbrennan@g.harvard.edu

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12 **Abstract**

13 The chemical and physical properties of the interiors of terrestrial planets are largely
14 determined during their formation and differentiation. Modeling a planet’s formation provides
15 important insights into the properties of its core and mantle, and conversely, knowledge of those
16 properties may constrain formational narratives. Here, we present a multi-stage model of Martian
17 core formation in which we calculate core–mantle equilibration using parameterizations from
18 high pressure–temperature metal–silicate partitioning experiments. We account for changing
19 core–mantle boundary (CMB) conditions, composition-dependent partitioning, and partial
20 equilibration of metal and silicate, and we evolve oxygen fugacity (fO_2) self-consistently. The
21 model successfully reproduces published meteorite-based estimates of the bulk silicate Mars
22 composition. This composition implies that the primordial material that formed Mars was
23 significantly more oxidized (0.7–1.4 log units below the iron–wüstite buffer) than that of the
24 Earth, and that core–mantle equilibration in Mars occurred at 45–91% of the evolving CMB
25 pressure. On average, at least 85% of accreted metal and at least 30% of the mantle were
26 equilibrated in each impact, a significantly higher degree of metal equilibration than previously

27 reported for the Earth. The modeled Martian core is rich in sulfur (16–20 wt%), with less than
28 one weight percent O and negligible Si.

29 We have used these core and mantle compositions to produce physical models of the present-
30 day Martian interior and evaluate the sensitivity of core radius to crustal thickness, mantle
31 temperature, core composition, core temperature, and density of the core alloy. Trade-offs in
32 how these properties affect observable physical parameters like planetary mass, radius, moment
33 of inertia, and tidal Love number k_2 define a range of likely core radii: 1620–1820 km. Seismic
34 velocity profiles for several combinations of model parameters have been used to predict seismic
35 body-wave travel times and planetary normal mode frequencies. These results may be compared
36 to forthcoming Martian seismic data to further constrain core formation conditions and
37 geophysical properties.

38 **1. Introduction**

39 In the absence of extensive seismic observations like those made available on Earth, our
40 knowledge of the Martian interior relies largely on interpreting measurable geophysical
41 properties, such as mass, radius, moment of inertia, and tidal responses, to constrain the depths,
42 densities, and compositions of the rocky and metallic layers of the planet. While the ongoing
43 InSight mission may directly measure the seismic properties of the interior (Panning et al.,
44 2017), interpreting these data will require an understanding of the Martian composition.

45 The most detailed information about the chemistry of the Martian interior comes from
46 extrapolating the compositions of the Martian meteorites, particularly the Shergotty-Nakhla-
47 Chassigny (SNC) group, back to their mantle source. Dreibus and Wänke (1985) developed a
48 canonical model for the silicate Mars (updated by Taylor, 2013) by measuring SNC elemental

49 abundances and proposing that their ratios reflect a mixture of volatile-rich and volatile-poor
50 source material. In later studies, such as those of Lodders and Fegley (1997) and Sanloup (1999),
51 compositional models were constructed by matching the oxygen isotopic composition of the
52 SNCs to mixtures of known meteorite types. From these studies, Mars is interpreted to have a
53 mantle enriched in iron oxide (FeO) and a smaller core mass fraction relative to Earth, indicating
54 more oxidizing formational conditions (e.g., Rubie et al., 2011). The proximity of Mars to the
55 protoplanetary snow line during its formation may have resulted in accretion of a larger portion
56 of relatively oxidized, volatile-rich material. Mars is also thought to have a core enriched in
57 sulfur, based on mass balance arguments (e.g., Anderson, 1972) and chalcophile element
58 depletions (Wänke and Dreibus, 1988). Addition of sulfur to iron significantly decreases its
59 melting temperature, so a high S content may have prevented crystallization of an inner core,
60 consistent with the lack of a modern geodynamo on Mars (Williams and Nimmo, 2004; Helffrich
61 2017).

62 One difficulty in evaluating the extant compositional models is determining whether they
63 accurately reflect the behavior of planetary materials during core formation. Single-stage core
64 formation models use metal–silicate partitioning data to determine a single pressure–
65 temperature–oxygen fugacity (P – T – fO_2) condition that can simultaneously reproduce the
66 Martian mantle abundances of several elements (e.g., Rai and van Westrenen, 2013; Righter and
67 Chabot, 2011; Steenstra and van Westrenen, 2018), but these models do not account for
68 changing conditions during planetary growth. Rubie et al. (2015) calculated Martian core
69 formation in a multi-stage model with self-consistent fO_2 evolution, though their model did not
70 include S and only used the Martian FeO content (in addition to Earth’s mantle composition) as a
71 constraint.

72 The core formation process on Mars has implications for the modern-day physical state
73 of the planet's interior. Previous studies developed models of the Martian interior that match
74 geophysical parameters such as the bulk density and moment of inertia factor (MOI), and
75 geochemical properties inferred from the SNC meteorites. Sohl and Spohn (1997) developed one
76 model that matched the MOI and another that matched the Fe/Si ratio of Mars. These models
77 improved on earlier assessments by using equations of state to calculate the behavior of Martian
78 minerals at high pressure and temperature and constrained the core size to 1400–1700 km.
79 Bertka and Fei (1998) found a core size compatible with the range of Sohl and Spohn (1997) for
80 Fe–14wt%S (~1400 km). Later measurements of the MOI of Mars, its tidal Love number (k_2),
81 and tidal dissipation factor (Q) seemed to only be matched by models with larger cores. For
82 example, Rivoldini et al. (2011) found that MOI and k_2 were best matched by cores 1730–1860
83 km in radius. Varying parameters such as the density of the core and the thermal structure of the
84 mantle can produce models that match these same constraints at a range of core sizes (Nimmo
85 and Faul, 2013), so it is important to evaluate the influence of these parameters. Khan et al.
86 (2018) inverted for the most likely ranges of several properties, including core composition,
87 core–mantle boundary (CMB) temperature, and lithospheric thickness, and they constructed
88 seismic velocity profiles based on these ranges. These results also suggest a large core (1730–
89 1840 km), though their Bayesian method does not explicitly consider the influence of each
90 parameter on the determined core size. Larger cores necessarily have more moderate lowermost
91 mantle pressures, probably precluding a region of bridgmanite stability, though Bertka and Fei
92 (1997) determined that the existence of Martian bridgmanite is also highly temperature
93 dependent.

94 Here we present a new model of Martian core formation, which improves upon previous
95 studies by implementing multi-stage differentiation with comparisons to a large suite of major,
96 minor, and trace elements in Mars. The core and mantle compositions predicted by this core
97 formation model were used to construct mineralogical, density, and seismic velocity profiles for
98 the Martian interior. We explicitly considered how planetary structure is influenced by core
99 composition as well as geophysical parameters such as crustal thickness and thermal structure.
100 Additionally, we introduced more realistic calculations of liquid Fe–S alloy densities at high
101 pressures and temperatures, improving our understanding of the core’s physical properties.
102 Seismic properties were assessed across the model suite, allowing predictions of both the body
103 wave travel times and normal mode oscillation frequencies for the different models. The new
104 self-consistent models of core formation, internal structure, and seismic properties presented here
105 help tie together the history of early Mars with its modern state and produce geophysical
106 predictions that can be compared to seismic results obtained by the InSight mission.

107 **2. Methods**

108 We have constructed a model of multi-stage core formation to investigate Martian
109 formational properties and a model of planetary physical structure to investigate geophysical
110 properties of modern Mars. Further details on each of these, as well as a description of our
111 seismological calculations, can be found in the supplementary materials.

112 2.1 Core formation

113 Chondritic primordial material was equilibrated at a fixed fO_2 to form planetesimals, then
114 these planetesimals were sequentially added to the proto-Mars, and experimentally-determined
115 metal–silicate partitioning data (Supplementary Table S1) were used to model the chemistry of

116 core formation. The composition of the primordial material was based on CI chondrites (after
117 Dreibus and Wänke, 1985; Taylor, 2013), enhanced in refractory elements (Mg, Al, Si, Ca, V, Cr,
118 Fe, Co, Ni, W, Ti) by a factor of 1.9 (Taylor, 2013) to create relative depletions in moderately
119 volatile elements (Na, P, S, K, Mn). Mars was constructed from 1,000 Ceres-sized ($0.001 M_{\text{Mars}}$)
120 planetesimals.

121 In each accretionary step, one planetesimal (the impactor) was equilibrated with the
122 proto-Mars (the target). Equilibration took place between the entire impactor mantle, a portion of
123 the impactor core, and a portion of the target mantle; the core of the proto-Mars was assumed to
124 be undisturbed by impacts. In each step, metal–silicate equilibration took place at a constant
125 fraction of the growing CMB pressure and at the liquidus temperature. Pressure at the CMB was
126 increased linearly from 1 GPa to 20 GPa (Rivoldini, 2011). Mg, Al, Ca, Na, K, and P were
127 assumed to be perfectly lithophile. In each step, major elements Si, Fe, O, and Ni were
128 partitioned first, allowing $f\text{O}_2$ to evolve self-consistently following the methodology of Rubie et
129 al. (2011) as updated in Fischer et al. (2017), then trace elements and S were partitioned. Finally,
130 the unequilibrated portion of the impactor core and the metallic portion of the equilibrated
131 material were added to the proto-Martian core, and the unequilibrated portion of the target
132 mantle and the silicate portion of the equilibrated material were combined to form the proto-
133 Martian mantle. This procedure was repeated for each impacting planetesimal.

134 Adjustable parameters in the model include: the equilibration fraction (the portion that
135 participates in the metal–silicate reaction) of the impactor core (denoted k) and target mantle;
136 depth of equilibration, expressed as a fraction of the evolving CMB pressure (denoted
137 $P_{\text{equil}}/P_{\text{CMB}}$); and the initial oxidation state of accreted material. To evaluate the sensitivity of the
138 resulting core and mantle compositions to these formational parameters and to constrain them,

139 the equilibration fractions of the impactor core and target mantle were each varied in the range
140 0.1–1.0, the depth of equilibration was varied in the range 0.01–1.0, and the initial fO_2 of the
141 accreted material was varied from IW–3 to IW. Uncertainties were evaluated using a Monte
142 Carlo analysis.

143 2.2 Physical structure

144 Using the core and mantle compositions calculated in the core formation model, radial
145 profiles of density and seismic wave speeds were constructed. The Martian temperature profile
146 (the “aerotherm”) was calculated based on an adiabat from the median CMB conditions of
147 Rivoldini et al. (2011) (~20 GPa and ~2000 K). These conditions correspond to a mantle
148 potential temperature of 1600 K, consistent with previous estimates (e.g., Nimmo and Faul,
149 2013; Zheng et al., 2015). The lithospheric thermal boundary layer was approximated as a layer
150 of linearly increasing temperature which intersects the adiabat at ~200 km, the estimated base of
151 the thermal boundary (e.g., Khan et al., 2018).

152 The Martian core was assumed to be a homogenous liquid alloy in the Fe–S system, with
153 the S fraction specified by the core formation model. Density–pressure relationships for the core
154 were calculated by reference to published equations of state for Fe–S alloys. The core S content
155 is a function of the formational parameters discussed above, so it was necessary to interpolate
156 between equations of state for several alloys to calculate densities over a range of compositions.
157 We used four equations of state: γ -Fe (Komabayashi and Fei, 2010), Fe_3S (Seagle et al., 2006),
158 FeS (Urakawa et al., 2007), and FeS_2 (Thompson et al., 2016). These equations of state all
159 describe solids, so it was necessary to correct for the difference in density between these and
160 liquid alloys. While it would have been more straightforward to use liquid equations of state,
161 there are not enough data to adequately constrain liquid Fe–S alloy densities over a range of

162 compositions (Section 4.4). Each constructed density and velocity profile of Mars corresponds to
163 a specific set of physical (crust thickness, mantle temperature, core temperature, volume change
164 (ΔV) of melting of Fe–S alloys) and formational (initial fO_2 , volatile loss, equilibration depth,
165 degree of equilibration) parameters. To test the sensitivity of core radius and density/velocity
166 structure to these parameters, crust thickness was varied in the range 25–85 km, mantle potential
167 temperature was varied in the range 1500–1800 K, the temperature contrast across the CMB was
168 taken to be 0–600 K, and ΔV of melting was taken to be 2–5%. Each combination of parameters
169 implies a value for the MOI and k_2 , which can be compared to the values measured by Mars-
170 orbiting satellites (Konopliv et al., 2011, 2016) (Section 4.4).

171 **3. Martian core formation**

172 The composition of the Martian mantle, as inferred from SNC meteorites, can be used to
173 constrain the conditions of core formation. The core formation conditions implied by the mantle
174 composition can then be used to place constraints on the composition of the core.

175 3.1 Mantle composition and implications for the formation of Mars

176 An example of a Martian mantle composition produced by this model is shown in Figure
177 1. Of the previous studies on Martian mantle composition, we primarily compare our results to
178 those of Taylor (2013) due to that study’s reporting of uncertainties, which other studies lack
179 (e.g. Dreibus and Wänke, 1985; Lodders and Fegley, 1996; Sanloup, 1999). The composition
180 predicted by this study best matches those of Taylor (2013) (Figure 1) and Dreibus and Wänke
181 (1985) due to use of the same bulk composition (Section 2.1). We obtain good agreement with
182 Lodders and Fegley (1996) and Sanloup (1999) when we instead use their bulk compositions.
183 Within uncertainty, calculated mantle abundances of most major, minor, and trace elements are

184 consistent with those of Taylor (2013), except for Cr and K (Figure 1). The anomalously low
185 concentration of Cr might arise because we are extrapolating beyond the fO_2 conditions of the
186 metal–silicate partitioning experiments. Taylor (2013) obtained the mantle K abundance from
187 gamma ray spectroscopy measurements of the surface K/Th ratio; this difference in methodology
188 likely accounts for the discrepancy in K. To constrain conditions of the formation and
189 differentiation of Mars, first the fO_2 at which the primordial material equilibrated was adjusted to
190 match the reported FeO content of the Martian mantle. The mantle FeO content implies that
191 Mars was built of material with an initial oxidation of state of IW–1.4 to IW–0.7, which
192 corresponds to a core mass fraction for Mars of 0.18–0.27 (Figure 2a). This higher fO_2 and
193 relatively smaller core than Earth (e.g., Rubie et al., 2011, 2015; Fischer et al., 2017) reflects the
194 accretion by Mars of relatively oxidized primordial material, which likely originated further from
195 the Sun.

196 Constraints on the degree of equilibration were obtained by comparing the calculated
197 mantle compositions with literature values, as shown in Figure 3a. Possible values of k are found
198 to be 0.84–1.0 for whole-mantle equilibration, based on matching the mantle abundances of
199 TiO_2 , S, and Co; other elements are consistent with this range but do not provide such tight
200 constraints. This degree of metal equilibration is significantly higher than that found for Earth by
201 examining the variation of mantle trace elements and the Hf–W isotopic system, which imply
202 that k for Earth is 0.2–0.55 (e.g., Fischer and Nimmo, 2018; Fischer et al., 2017). A lower k for
203 Earth is consistent with the accretion of giant differentiated impactors, whose large cores would
204 not have efficiently emulsified. Mars' high k is consistent with the accretion of smaller
205 impactors, possibly including undifferentiated ones that would exhibit $k \sim 1$. Varying the
206 equilibration fraction of the target silicate does not significantly change the mantle composition

207 for values above ~ 0.3 , consistent with its limited effect on composition above a certain threshold
208 for the Earth (Fischer et al., 2017). Reducing the degree of silicate equilibration requires a
209 corresponding increase in k ; since k is already near unity (its maximum value) for the case of
210 whole-mantle equilibration, it is more likely that silicate equilibration was similarly high.

211 An analogous procedure was used to constrain the depth of metal–silicate equilibration
212 (Figure 3b). Simultaneously matching the Martian mantle abundances of Ni, Co, and S requires
213 that $P_{\text{equil}}/P_{\text{CMB}}$ fall in the range 0.40–0.91 (for $k = 0.9$ and whole-mantle equilibration); again,
214 other elements are consistent with this range, but do not further constrain it. This pressure range
215 implies that, on average, equilibration took place in a deep magma ocean but not as deep as the
216 core–mantle boundary. It overlaps with the relative depth of equilibration found for the Earth
217 using similar models (Fischer et al., 2017; Rubie et al., 2011, 2015), which may suggest a similar
218 relative depth of melting on the two planets. Applying this range to the modern Martian CMB
219 implies an average equilibration pressure of ~ 13 GPa, similar to the results of single-stage
220 partitioning studies (e.g., Rai and van Westrenen, 2013; Righter and Chabot, 2011). Single-stage
221 models necessarily partition elements at a fixed $f\text{O}_2$ and do not incorporate changes in pressure
222 and temperature as a planet grows, so the model presented here represents a more realistic
223 approach.

224 3.2 Light elements in the Martian core

225 The core formation conditions implied by the Martian mantle composition indicate that S
226 is the dominant light element in the core, consistent with previous studies (e.g., Lodders and
227 Fegley, 1996; Sanloup et al., 1999; Steenstra and van Westrenen, 2018; Taylor, 2013; Wänke
228 and Driebus, 1985). Sulfur is siderophile at the P – T – $f\text{O}_2$ conditions of Martian core formation,
229 with D_S values as high as 600, comparable to D_{Ni} (Fischer et al., 2015). The majority of Martian

230 S must be in the core, but the mantle abundance also appears to be greater than that of the Earth
231 (e.g., Wang and Becker, 2017), implying that bulk Mars is relatively sulfur-rich. The range of
232 core mass fractions implied by the mantle FeO content, 0.18–0.25 (Section 3.1), is consistent
233 with a range of volatile element depletion factors of 0.28–0.68× CI (Figure 2b). Taylor (2013)
234 argued for a refractory element enrichment of 1.9× CI (equivalent to a volatile element depletion
235 of 0.6× CI) based on a survey of lithophile volatile element abundances in Mars. Enriching Mars
236 in refractory elements by this factor leads to a core S content of 18 wt%, with the uncertainty of
237 the Monte Carlo analysis expanding this to a preferred range of 16–20 wt% (95% confidence
238 interval; Supplementary Table S2). This corresponds to a bulk Mars with 4.2 wt% S, within the
239 bulk abundance estimates of Steenstra and van Westrenen (2018). If Mars instead is assumed to
240 have bulk S equivalent to an H chondrite, it would have a core S content of 12 wt%. Bulk S
241 content equivalent to a pristine EH chondrite results in a core S content of 21 wt%; this may be
242 taken as the upper limit for core S in a chondritic Mars since EH is the most S-rich of all
243 chondrite groups (Lodders and Fegley, 1998).

244 The Martian core contains little O (<1 wt%; Supplementary Table S2) despite the more
245 oxidizing core formation conditions compared to the Earth. This is largely due to the less
246 extreme conditions of metal–silicate equilibration on Mars, since O partitions more strongly into
247 iron alloys at higher T (e.g., Fischer et al., 2015). Previous studies which predicted O at the few-
248 percent level in the Martian core (e.g., Steenstra and van Westrenen, 2018) calculated
249 partitioning at modern lowermost mantle conditions (inconsistent with our findings; Figure 3b).
250 The other light element considered here, Si, only enters the Martian core at trace levels
251 (Supplementary Table S2). Like O, it is less siderophile at lower temperatures, but it is also less
252 siderophile at higher fO_2 (e.g., Fischer et al., 2015), further reducing its core abundance.

253 C or H partitioning into the core were not modeled despite suggestions that these may be
254 present in greater-than-trace abundances (e.g., Chi et al., 2014; Zharkov and Gudkova, 2005).
255 There are few constraints on the planetary or mantle abundances of these highly volatile
256 elements, and thus it is difficult to determine their total budgets. Qualitatively, Mars is too small
257 and S-rich to dissolve substantial H in its core, with Clesi et al. (2018) estimating 60 ppm. The
258 solubility of C is also much reduced in S-rich core alloys (Tsuno et al., 2018). For a nominal
259 bulk C content of 1000 ppm, Tsuno et al. (2018) found that a Martian core at IW-1.0 with 16
260 wt% S would have ~0.5 wt% C; this may be taken as an upper bound for the more S-rich core
261 composition presented here. Better constraining the abundances and partitioning of these highly
262 volatile elements is a target for future studies.

263 **4. Geophysical properties of Mars**

264 The core and mantle compositions predicted by the core formation model were used to
265 construct phase assemblages (Supplementary Figure S1) and produce density and velocity
266 profiles (Figures 4 and 5) of the Martian interior. In addition to composition, these profiles
267 depend on physical properties of the Martian interior. By comparing to the mass, radius, MOI,
268 and k_2 , constraints can be placed on some of Mars' geophysical properties. The resulting solution
269 space allows for predictions of core radii and seismic properties.

270 4.1 The lithospheric boundary layer

271 The rigid lithosphere at a planet's surface does not participate in mantle convection, so its
272 heat flow is conductive, with temperatures increasing approximately linearly with depth. On
273 Earth, this rapidly increasing temperature leads to high seismic velocities in the conductive lid
274 and a corresponding low-velocity zone (LVZ) in the uppermost adiabatic mantle. Mars is a

275 stagnant lid planet and is inferred to have a laterally variable lithosphere up to 300 km thick (e.g.,
276 Grott et al., 2013). This produces a thick thermal boundary layer on a small planet, so the low-
277 velocity effect which confined to a small portion of the Earth's mantle will extend over a
278 sizeable portion of the Martian mantle. As seen in Figure 5, this may be a property of first-order
279 importance for Martian seismology (Section 4.6). Since the magnitude of the decrease is
280 dependent on the thermal structure of the lithosphere, mantle potential temperatures may be
281 inferred by measuring the LVZ's seismological effects (Zheng et al., 2015).

282 The magnitude of this effect, however, cannot be well-constrained with our current
283 knowledge of Martian temperature and structure. The calculations shown here use an upper
284 mantle thermal boundary layer thickness of 200 km (Khan et al., 2018) and a range of mantle
285 potential temperatures around 1600 K (Nimmo and Faul, 2013). Lithospheric thickness directly
286 influences the size of the LVZ, but also reduces its magnitude, since a deeper thermal boundary
287 would be shallower and closer in slope to the mantle adiabat. Changing the mantle potential
288 temperature at a constant lithospheric thickness likewise requires changing the slope of the
289 lithospheric temperature profile (Supplementary Figure S2). Increasing potential temperature by
290 100 K for a 200 km lithospheric boundary increases the magnitude of the LVZ by 0.2 km/s for
291 compressional waves and 0.1 km/s for shear waves. These effects may be complicated by lateral
292 variations in lithospheric thickness due to features such as the hemispherical dichotomy and the
293 Tharsis volcanic province.

294 4.2 Lowermost mantle conditions

295 There is some disagreement as to whether the Martian mantle contains bridgmanite, the
296 major component of Earth's lower mantle. Some studies find that the P - T conditions of the
297 lowermost Martian mantle lie within the bridgmanite stability field (e.g., Bertka and Fei, 1998),

298 some do not (e.g., Sohl and Spohn, 1997; Khan and Connolly, 2008; Khan et al., 2018), and
299 several are inconclusive (e.g., Bertka and Fei, 1997; Rivoldini et al., 2011). At a lower mantle
300 temperature of 2000 K, the parameterization of Fei et al (2004) suggests that bridgmanite
301 becomes stable at 22.9 GPa. This CMB pressure corresponds to a core radius of approximately
302 1500 km; such a core is smaller than any in Figure 4, but it could be produced by, for example, a
303 low S content, a shallow crust, and no CMB thermal boundary layer. Such a small core is
304 difficult to reconcile with geophysical constraints (see Section 4.4). The bridgmanite stability
305 field grows with temperature, so a hot lower mantle might support bridgmanite at slightly lower
306 pressures. At 2500 K, bridgmanite becomes stable at 22.2 GPa, corresponding to a 1570 km
307 core; such temperatures could only be produced by a CMB thermal boundary layer with a large
308 temperature contrast. This would tend to increase the core radius well beyond this size, meaning
309 that it seems unlikely that bridgmanite exists within modern Mars. A bridgmanite layer would
310 affect mantle convection, increase the temperature of the lower mantle, and reduce heat flow
311 from the core, impacting the both the areochem and the contrast across a CMB thermal boundary
312 layer (Bruer et al., 1998; Michel and Forni, 2011). Thus, if a bridgmanite layer does exist, its
313 thickness will strongly constrain mantle temperature (Bertka and Fei, 1997); the possibility of
314 such a layer in Mars' hotter past may have influenced the convective regime of the Martian
315 mantle towards single-plume upwelling (Sohl and Spohn, 1997).

316 4.3 The crust

317 The outer layers of a planet have an outsized influence on the planet's MOI due to their
318 large radial distance from the center of gravity. Konopliv et al. (2011) determined the Martian
319 MOI to be 0.3644 ± 0.0005 but found that altering crustal thickness by 25 km changes the MOI
320 by 0.0017. Therefore, uncertainties in crustal structure dominate the inertia-based constraints on

321 models of the Martian interior. Some recent studies use an even tighter bound on MOI (Khan et
322 al, 2018). Determining the average crustal properties pertinent to a spherically-symmetric model
323 is complicated by the fact that the Martian crust contains a significant dichotomy between the
324 northern and southern hemispheres, various volcanic provinces, impact basins, and
325 heterogeneous regolith. Constraints from orbital gravity measurements and surface topography
326 imply that mean crustal thickness must lie within 57 ± 24 km (Wieczorek and Zuber, 2004), with
327 some studies preferring different portions of this range. We find that within a narrow range of
328 crust sizes (55 ± 10 km) the Martian MOI can be matched with a wide range of core sizes (1500–
329 1850 km). Fortunately, InSight measurements are likely to strongly constrain crustal thickness
330 beneath the landing site (Panning et al., 2017), which will allow for tighter constraints on core
331 size.

332 4.4 Core radius

333 We have evaluated the effects of five parameters on the core radius of Mars: the
334 thickness of the crust, temperatures of the mantle and core, sulfur content of the core, and
335 densities of liquid Fe–S alloys. All core radii calculated here are consistent with the core mass
336 fraction range determined in the core formation model (Section 3.1; Figure 2).

337 (1) Thickness of the crust. A thick layer of relatively light crustal material requires a
338 larger core to maintain consistency with the Martian radius and bulk density. Varying
339 the crustal thickness in the range 25–85 km (Wieczorek and Zuber, 2004)
340 corresponds to a change in core radius of 94 km, with thicker crusts corresponding to
341 larger cores. The planet’s MOI is very sensitive to crustal parameters, so only a small
342 portion of this range of crust thicknesses is consistent with measurements (Section
343 4.3).

344 (2) Temperature of the mantle. Martian internal temperature profiles depend on the
345 thermal history of the planet, its radiogenic heat production, and its convective
346 regime. These features are not well constrained, making temperatures difficult to
347 evaluate. Lowermost mantle temperatures of 1800–2100 K bracket the “hot” and
348 “cold” endmembers of Rivoldini et al. (2011). This range corresponds to mantle
349 potential temperatures of 1500–1800 K, consistent with published estimates (e.g.,
350 Nimmo and Faul, 2013). This temperature range corresponds to a change in core
351 radius of 122 km, with larger cores corresponding to hotter mantles.

352 (3) CMB thermal boundary layer. Previous studies (e.g., Khan et al., 2018) have
353 generally not considered any significant temperature change across the CMB due to
354 the absence of a Martian geodynamo (Williams and Nimmo, 2004). It is possible that
355 the core is hotter than the overlying mantle, leading to a thin region of rapidly
356 increasing temperatures, analogous to Earth’s lowermost mantle. We have
357 investigated models with uppermost core temperatures ranging from 0–600 K above
358 the lowermost mantle temperature, within the allowable range of CMB heat flow (see
359 supplementary materials for more details). This range corresponds to a change in core
360 radius of 103 km, with hotter cores being less dense and thus larger.

361 (4) Sulfur content of the core. Since S is much lighter than Fe, a core with a large S
362 component will have a reduced alloy density, and thus must be larger. Our
363 compositional results (Section 3.2) indicate that to maintain consistency with the
364 inferred mantle composition, the Martian core contains 16–20 wt% S; this range
365 corresponds to 65 km of variability in core size. A core S content of 12–21 wt%
366 encompasses the range of 2.0–5.4 wt% bulk Martian S, corresponding to the

367 difference between the most S-poor (H) and S-rich (EH) chondrites (Lodders and
368 Fegley, 1998). This range changes core radius by 141 km.

369 (5) Effect of melting on Fe–S alloy densities. Since the Martian core is thought to be
370 entirely molten (Konopliv et al., 2011), its geophysical parameters must be calculated
371 with reference to liquid Fe–S alloys. Unfortunately, there are few equation of state
372 studies in this liquid system, and the available ones do not generally extend to the
373 relevant P – T conditions. Some previous studies (e.g., Rivoldini et al., 2011; Khan et
374 al., 2018) have attempted to overcome this difficulty by extrapolating the extant
375 liquid data, but this may underestimate the true density (Figure 6). Several equation
376 of state studies have pointed out that the ΔV between solid and liquid Fe–S alloys
377 should be quite small at high pressures, on the order of 1.5% for the Earth’s CMB
378 (Seagle et al., 2006) and only slightly greater for Martian CMB conditions. The
379 ambient ΔV is $\sim 16\%$ for FeS (Kaiura and Toguri, 1979), dropping to only ~ 4 – 5% at a
380 few GPa (Nishida et al., 2011). For this study, we have chosen to use the interpolation
381 of the solid densities and correct for a melting effect based on the eutectic melting
382 curve of Fe–S alloys (Campbell et al., 2008), leading to a 3.6% ΔV of melting at the
383 Martian CMB that decreases at greater depth. We have also investigated the effect of
384 imposing fixed ΔV values from 2–5%. This range corresponds to a change in core
385 radius of 56 km.

386 One of the geophysical constraints on the Martian interior comes from its deformation in
387 response to tidal forcings from the Sun, Phobos, and Deimos. The tidal Love number k_2 has been
388 determined from spacecraft and lander tracking data, most recently in Konopliv et al. (2016),
389 which reported a value of 0.169 ± 0.006 . To evaluate the consistency between this value and our

390 profiles of the Martian interior, we used a simplified two-layer parameterization for calculating
391 k_2 (see supplementary materials for more details). The dissipation of tidal energy within Mars is
392 dependent on the rigidity of the core and mantle layers and their relative sizes. A liquid core
393 cannot sustain shear stress, so its rigidity is negligible; therefore, a very rigid mantle requires a
394 large core to match the planetary k_2 . This tradeoff indicates that, for example, a mean mantle
395 rigidity of $\mu = 80$ GPa requires a core 1840–1900 km in radius to match k_2 , while a softer mantle
396 with $\mu = 60$ GPa only requires a 1540–1640 km core (Supplementary Figure S3). If the Martian
397 mantle accurately reflects the volumetrically averaged shear modulus of ~ 73 GPa calculated
398 here, then the core should be 1740–1820 km in radius. It is possible to produce a core of at least
399 this size through several combinations of the parameters considered above, even accounting for
400 the constraint on crust size from MOI. The relationship between core radius and the geophysical
401 and geochemical parameters considered here is illustrated in Figures 7 and S4, and can be
402 parameterized by the following equation:

$$\begin{aligned} 403 \quad R_{core} = & 564 + 1.49 d_{crust} + 10.1 C_{core}^S + 0.183(C_{core}^S)^2 + 0.115 \Delta T_{TBL} \\ 404 \quad & + 0.000108 (\Delta T_{TBL})^2 + 0.423 T_P + 14.8 \Delta V_{core} + 0.337 (\Delta V_{core})^2 \end{aligned} \quad (1)$$

405 where R_{core} is the radius of the core (km), d_{crust} is the thickness of the crust (km), C_{core}^S is the S
406 content of the core (wt%), ΔT_{TBL} is the temperature contrast across the core–mantle thermal
407 boundary layer (K), T_P is the mantle potential temperature (K), and ΔV_{core} is the volume change
408 of melting associated with the core alloy (%; e.g., for a 2% volume change of melting, $\Delta V_{core} =$
409 2). This equation reproduces the results of our geophysical model with a root mean squared
410 misfit of 9 km for core radii of 1450–2000 km and the parameter ranges listed above and should
411 not be applied to more extreme cases. Future seismological constraints on crust thickness and

412 core radius can be inserted into this equation to help constrain geophysical properties of the
413 Martian interior.

414 It is also possible that the Martian mantle is less rigid than the melt-free anhydrous
415 idealization depicted here and by other studies. Shear moduli are significantly reduced by both
416 the presence of H and partial melts in mantle minerals. The 300 ppm water suggested to reside in
417 the Martian mantle (Taylor, 2013) would not significantly reduce the mean shear modulus, but
418 Martian water abundances are extremely uncertain. Partial melting is another possibility; fluids
419 cannot support shear stress, so partial melts would decrease the mean shear modulus by the same
420 amount as their volume fraction. Selecting a crust size of 55 km, a potential temperature of 1600
421 K, a core S content of 18 wt%, no TBL, and ΔV of melting of 3% returns a core 1620 km in
422 radius. To match k_2 , this core would require a mean mantle rigidity of 55 GPa, a 15% reduction
423 from our nominal value. This amounts to a basal magma ocean 500 km deep. Such a feature is
424 unlikely, but volumetrically significant melting may also occur beneath the Martian lithosphere
425 (Duncan et al., 2018). Ultimately, some combination of mantle-softening and core-expanding
426 parameters must be responsible for the observed Martian k_2 .

427 4.5 Density and velocity profiles of the Martian interior

428 We consider the effects of the same five geochemical and geophysical parameters (crust
429 thickness, core and mantle T , core S content, Fe–S ΔV of melting) on the density and velocity
430 structure of the Martian interior (Figure 4). Unlike some previously-modeled velocity profiles
431 (e.g., Khan and Connolly, 2008; Zharkov and Gudkova, 2009), we predict a low-velocity zone in
432 the upper mantle due to the steep lithospheric temperature gradient (Section 4.1). Our results
433 share many properties in common with previous LVZ models, such as the large contrast between
434 adiabatic and lithospheric temperatures (Nimmo and Faul, 2013) and a gradual olivine–

435 wadsleyite phase transition due to the high FeO content. This study predicts a V_S in the
436 lowermost mantle that is smaller than V_P at the top of the core, whereas the otherwise similar
437 LVZ model of Zheng et al. (2015) does not (Figure 5). The lower V_P of Zheng et al. (2015) is
438 likely due to their use of FeS data for the thermophysical properties of the core alloy; FeS has a
439 reduced density and bulk modulus compared to our more moderate composition.

440 4.6 Seismic properties

441 Mode center frequencies for the suite of models have been calculated (Figure 8a and S5).
442 Overall, as expected, radial, core-sensitive, and Stonely modes are affected by adjusting the five
443 parameters described above. Stonely modes are confined to the CMB and are very challenging to
444 observe even on Earth. Modes with center frequencies below 5 mHz are unlikely to be detectable
445 on Mars (Panning et al., 2017), but radial modes (on the left of Figure 8a) above this period may
446 display changes in frequency of several percent. While not affected by the physical properties of
447 the core itself, we note that models with different crustal thicknesses and mantle potential
448 temperatures will result in different frequencies for the fundamental modes, which are a target
449 for observation (Bissig et al., 2018). Thus, any observations of normal modes on Mars will aid in
450 discrimination between these different models of Martian formation.

451 Body wave travel times (Figure 8b) show that a range of phases that are reflected at the
452 CMB or travel through the core are sensitive to the parameters explored here. As all the models
453 investigated have an LVZ in the upper mantle (Section 4.1), shadow zones are evident in the
454 travel time curves, most prominently in the direct S phase. Models with larger cores show earlier
455 arriving core-reflected phases (for example ScS), whilst signals like PKP are delayed as V_P in the
456 core is lower than that of the mantle. SKS, which travels through the mantle as a shear wave and
457 through the liquid core as a compressional wave, has delay times that vary little though the

458 model suite as V_s in the mantle is very close to V_P in the core. If it can be observed, SKKS, which
459 transits the core twice, would be a better indicator of core size; SKKS's amplitude may be
460 insufficient to observe in InSight data however. Because V_P just below the CMB is higher than
461 V_S just above the CMB in our models, we predict the presence of minor arc SKKS at a wide
462 range of distances (Helffrich, 2017).

463 The InSight site is roughly 20° from Cerberus Fossae (Taylor et al., 2013). At such a
464 distance, one of the clearest core signals we hope to observe will be ScS. Figure 9 shows
465 predicted travel times for this phase at this epicentral distance for the full suite of core models.
466 Nearly all the parameters behave in the same way: shorter ScS travel times correspond to larger
467 core radii. Thus, even though all properties may not be discernable from such an observation, a
468 travel time should permit us to roughly estimate core radius in this framework. Mantle potential
469 temperature has effects on the radius–ScS time relationship which are not co-linear with the
470 other parameters because a hotter potential temperature both decreases mantle velocities and
471 changes core radius. Both crustal thickness and mantle potential temperature may be obtainable
472 from other seismological observables (e.g., receiver function analysis for the former, and
473 estimates of the sub-lithospheric LVZ for the latter), making this kind of analysis more valuable
474 as the possible parameter space is narrowed down further.

475 **5. Conclusions**

476 A multi-stage core formation model has successfully reproduced meteorite-based
477 compositions of the bulk silicate Mars and has been used to determine conditions of core
478 formation and the composition of the Martian core. The high FeO content of the Martian mantle
479 relative to that of Earth is due to formation from primordial material initially equilibrated at
480 approximately IW–1.25. On average, >85% of incoming metal was equilibrated with >30% of

481 the Martian mantle upon impact, and equilibration took place at a depth of 45–91% of the
482 evolving CMB pressure. The light element composition of the Martian core is dominated by S
483 (16–20 wt%), with <1 wt% O and negligible Si.

484 We have considered the possible ranges of various geophysical parameters (mantle and
485 core temperatures, crustal thickness, and density of the Fe–S core alloy) and evaluated the effects
486 of varying these parameters on the structure of the Martian interior. The core alloy densities
487 calculated here are somewhat higher than those of previous studies due to different
488 interpretations of the Fe–S equation of state data. Conservative parameter combinations imply
489 that the core could be as small as 1620 km, though this size is not consistent with geophysical
490 constraints on tidal Love number k_2 unless the Martian mantle is significantly softened by the
491 presence of melt or water. Larger values of the crustal thickness, mantle temperature, core
492 temperature, or S content imply larger cores (Equation 1). If the Martian mantle is not subject to
493 any softening effects, the core can be as large as 1820 km while maintaining consistency with
494 geophysical observations. We have calculated seismic phase arrival times and planetary normal
495 modes for a variety of parameter combinations to facilitate comparison with InSight’s upcoming
496 seismological measurements. Whatever the results of these observations, the actual core radius
497 implies a particular combination of geophysical and geochemical parameters, meaning that
498 constraints on core radius will help elucidate the thermal, physical, and compositional state of the
499 Martian interior.

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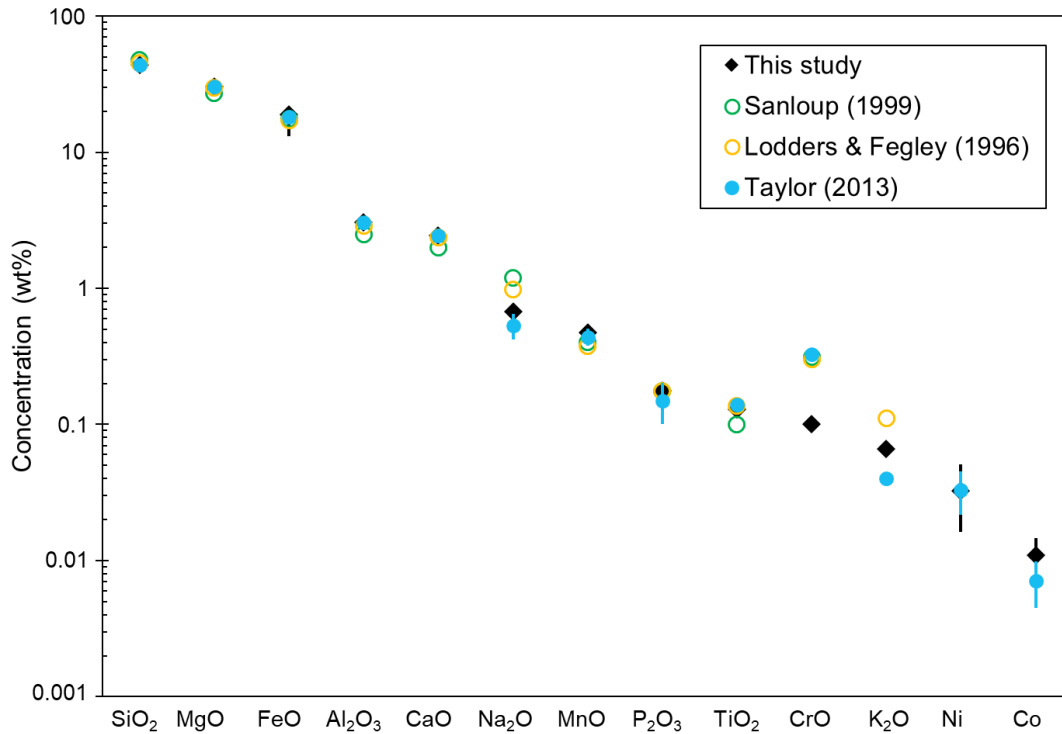
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530 **Figures**



531

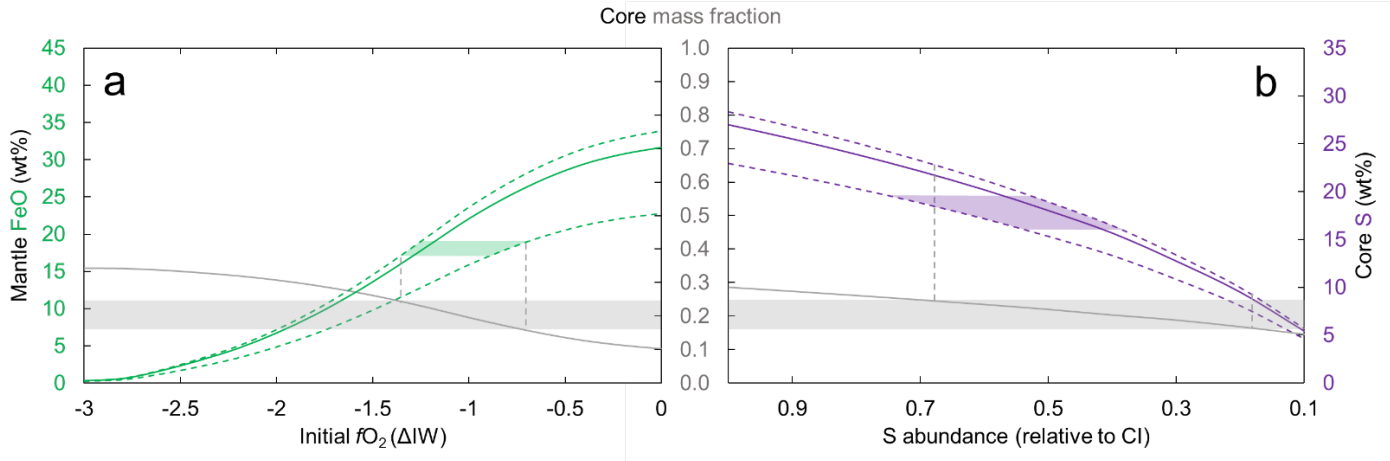
532 **Fig. 1.** Comparison of bulk mantle compositions between this study and models based on SNC
533 elemental abundances (Taylor, 2013) or O isotopes (Lodders and Fegley, 1996; Sanloup, 1999).
534 Error bars correspond to 95% confidence intervals of our Monte Carlo analysis for this study and
535 reported 2σ uncertainties for Taylor (2013). Calculation was performed for $k = 0.9$, whole mantle
536 equilibration, $P_{equil}/P_{CMB} = 0.66$, and initial fO_2 of IW-1.2.

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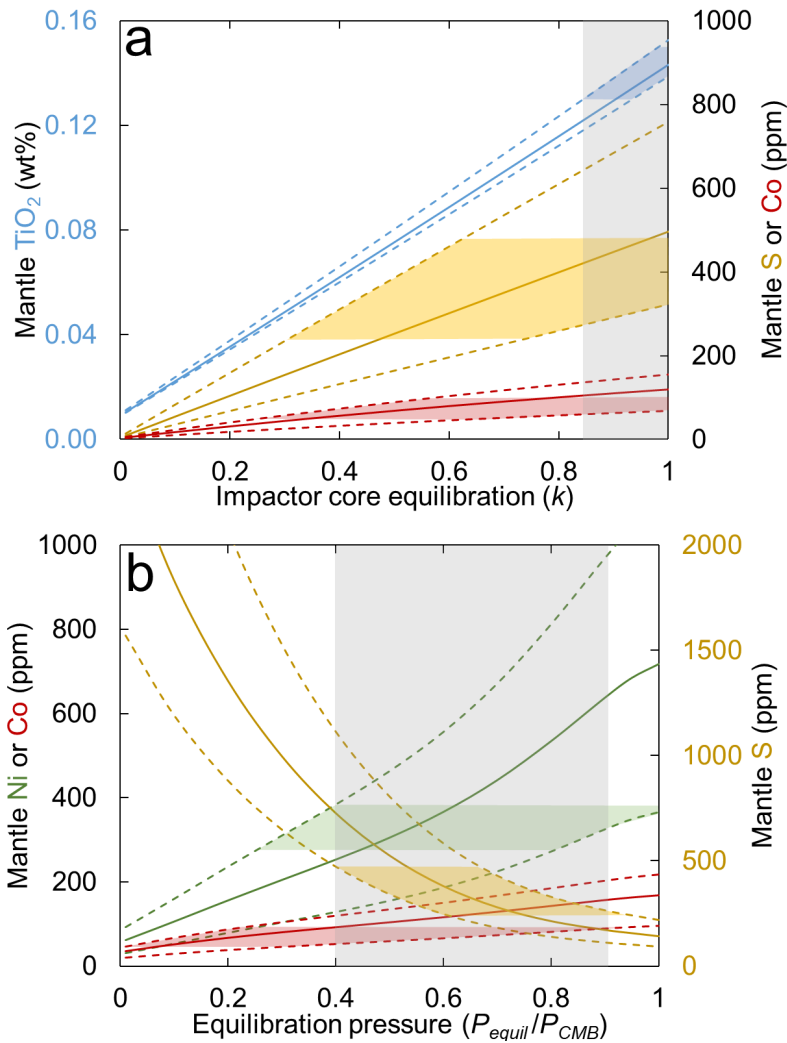
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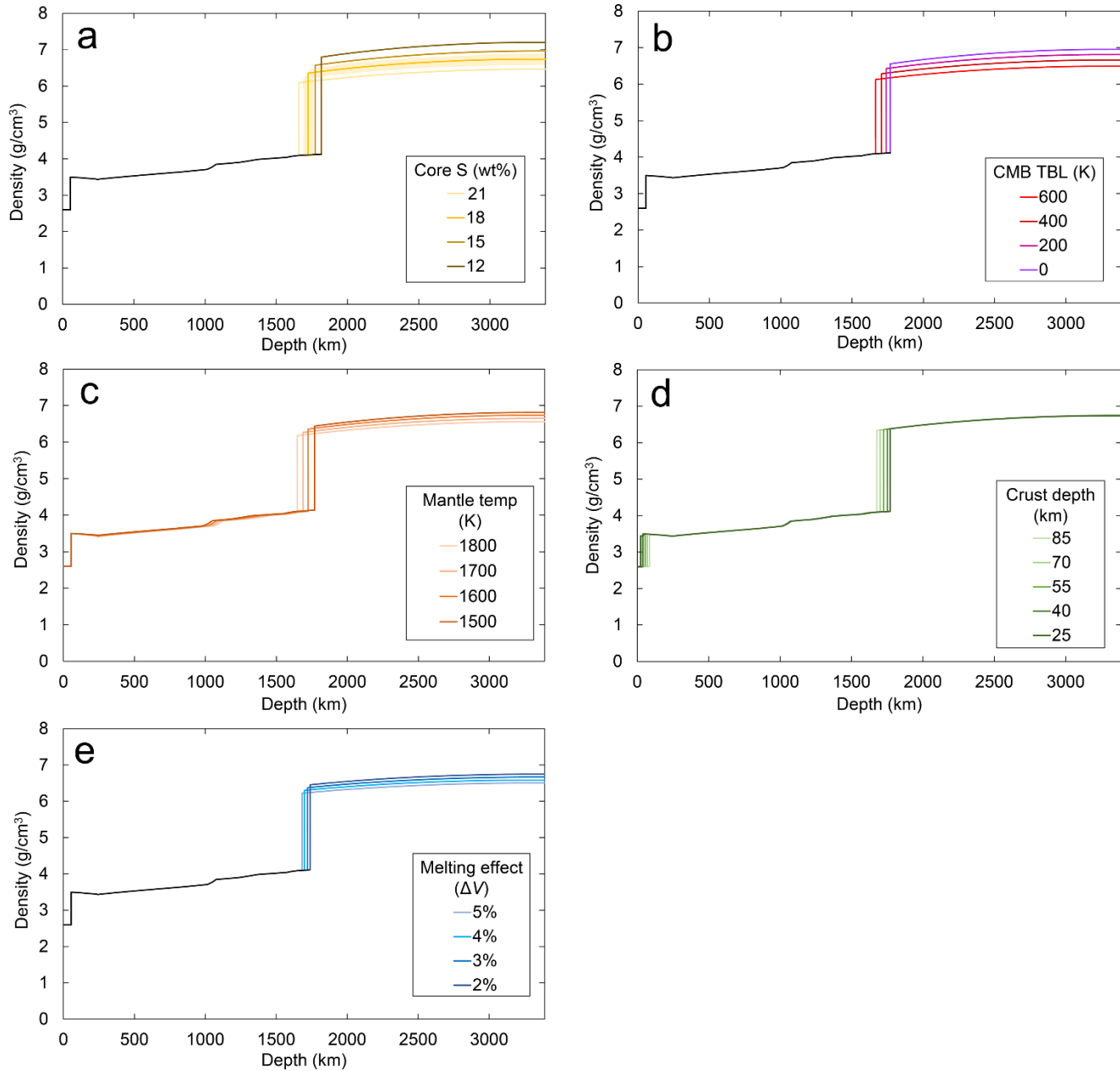
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542 **Fig. 2. a.** The tradeoff between the initial fO_2 of Mars' primordial material and the partitioning of
 543 Fe between mantle and core. The green shaded region indicates the range of calculated FeO
 544 contents that are consistent with Taylor (2013), which constrain the initial fO_2 to be ΔIW -0.7 to
 545 ΔIW -1.4. The corresponding core mass fraction is 0.17–0.26 (grey curve and grey horizontal
 546 shaded bar). **b.** The tradeoff between bulk S content and S content of the core (purple). For the
 547 same range of core mass fractions as in **a** (grey curve and grey horizontal shaded bar), the total S
 548 content of bulk Mars is constrained to be 0.20–0.68 \times CI. The purple shaded region represents
 549 the range of core S contents from the core formation model. Dashed lines represent 95%
 550 confidence intervals at $P_{equil}/P_{CMB} = 0.66$ and $k = 0.9$.



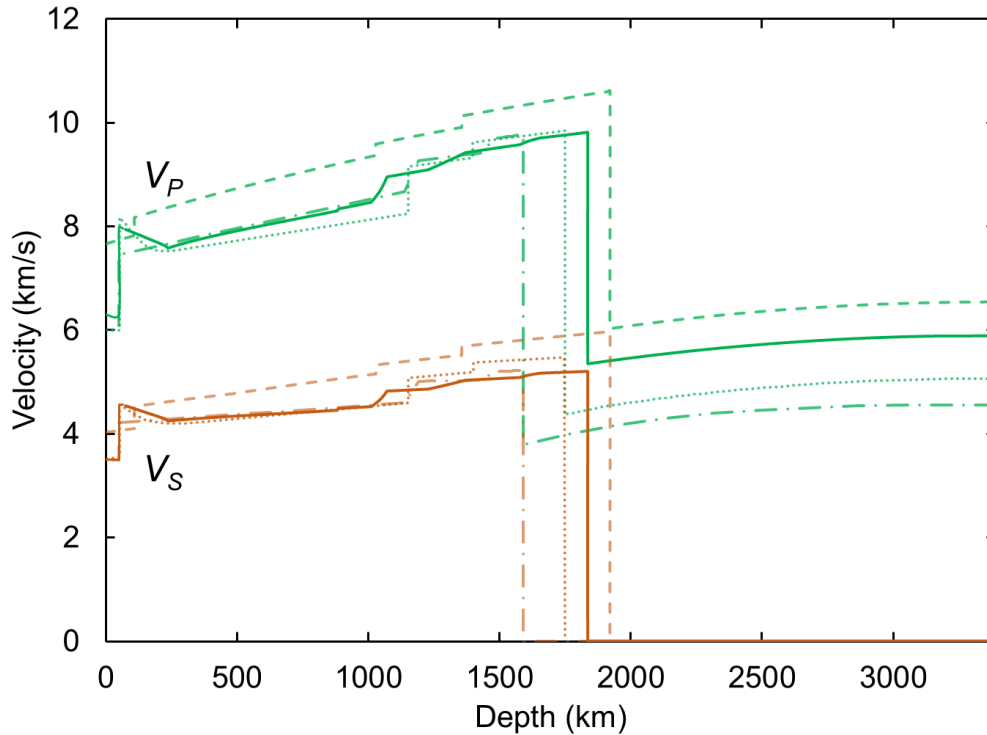
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552 **Fig. 3. a.** Variation in the mantle concentrations of TiO_2 (blue), Co (red), and S (yellow) as a
 553 function of the degree of impactor core equilibration, k . Dashed lines are 95% confidence
 554 intervals. The colored regions illustrate where the calculated compositions are consistent with the
 555 previously published values of Taylor (2013) for TiO_2 and Co, and Wang and Becker (2017) for
 556 S. The grey shaded bar indicates the range of k in which all three elements can be matched.
 557 These values of k suggest that most metal was emulsified and equilibrated before merging with
 558 the Martian core. Calculation was performed for whole mantle equilibration, $P_{\text{equil}}/P_{\text{CMB}} = 0.66$,
 559 and initial $f\text{O}_2$ of IW-1.2. **b.** Variations in the mantle concentrations of Ni (green), Co (red), and
 560 S (yellow) as a function of core-mantle equilibration pressure (expressed as a fraction of the
 561 evolving CMB pressure). The colored regions illustrate where the calculated compositions are
 562 consistent with the previously published values of Taylor (2013) for Ni and Co and Wang,
 563 and Becker (2017) for S. These values of equilibration pressure suggest that equilibration occurred in
 564 a deep magma ocean, but not at the core-mantle boundary. Calculation was performed for $k =$
 565 0.9, whole mantle equilibration, and initial $f\text{O}_2$ of IW-1.2.



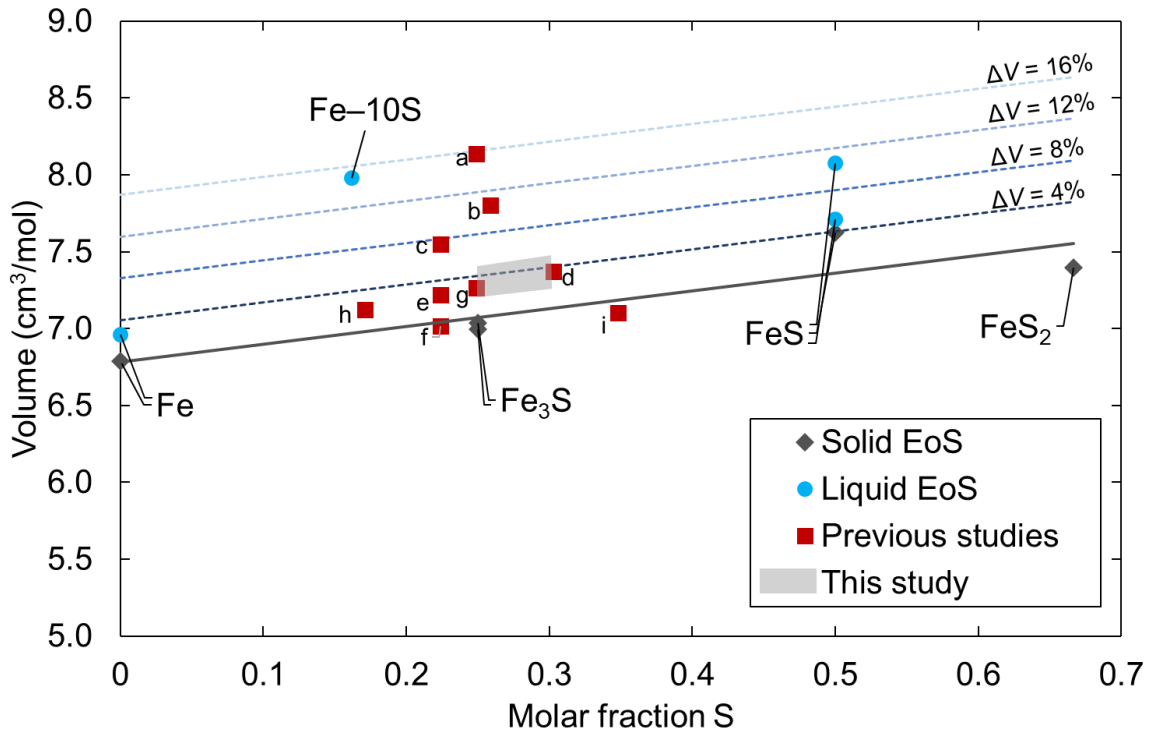
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 567 **Fig. 4.** Martian density profiles calculated by varying a single parameter at a time: core S content
 568 (a), temperature contrast between the lowermost mantle and uppermost core (assuming a thin
 569 thermal boundary layer at the CMB) (b), mantle potential temperature (c), crustal thickness (d),
 570 and ΔV of melting of Fe–S alloys (e). The shaded region in (a) corresponds to our preferred S
 571 range of 16–20 wt% from the core formation model at initial $fO_2 = IW-1.2$, $P_{equil}/P_{CMB} = 0.66$
 572 and $k = 0.9$ (Section 3.2).

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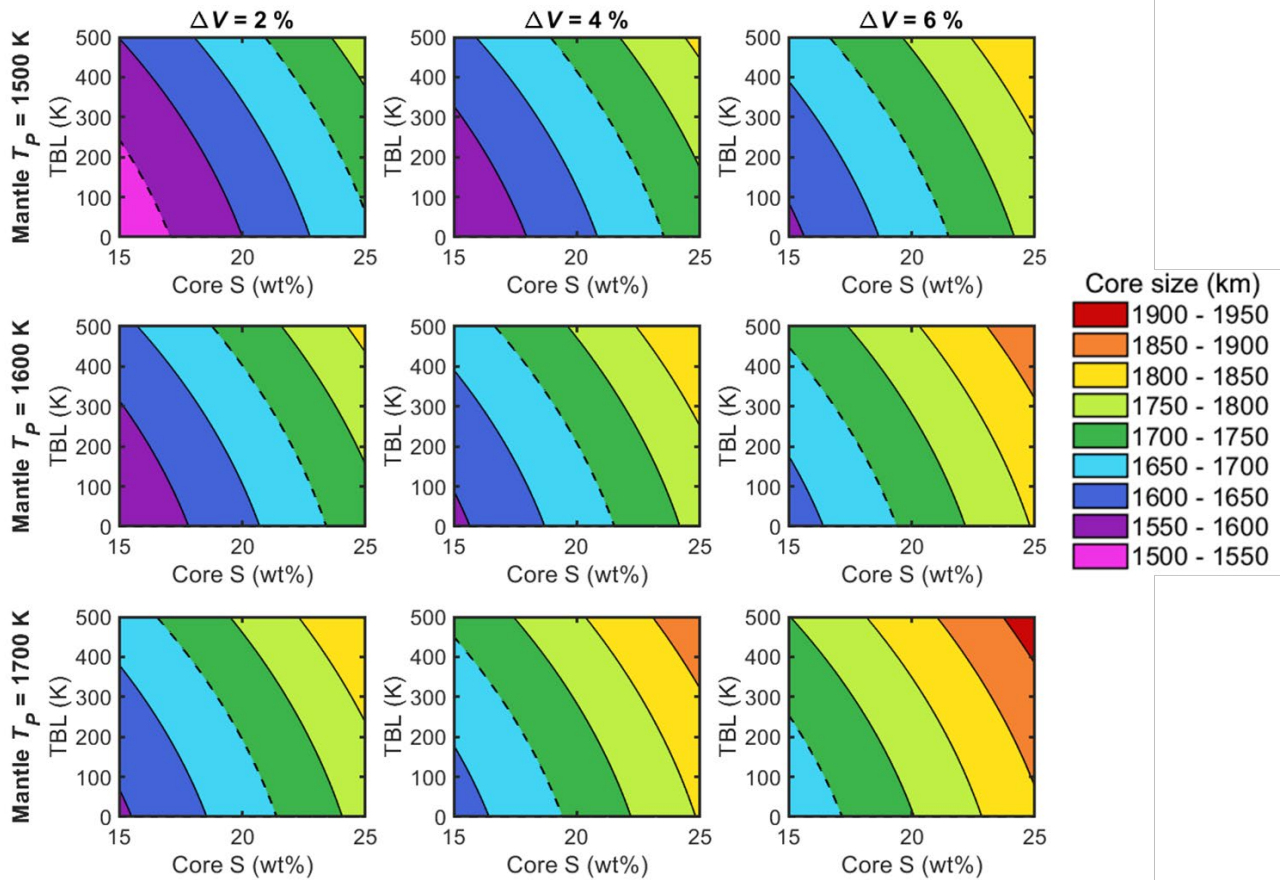
574 **Fig. 5.** Comparison of Martian compressional wave velocity (V_P) and shear wave velocity (V_S)
575 profiles between this and several previous studies (dashed line: Sohl and Spohn, 1997 “Model
576 A”; dotted line: Zheng et al., 2015 “LVZ Model”; dot-dashed line: Zharkov and Gudkova, 2009
577 “M14_3 Model”). The profile for this study corresponds to a core sulfur content of 18 wt%,
578 crustal thickness of 50 km, thermal boundary layer temperature contrast of 300 K, and mantle
579 potential temperature of 1600 K. The low-velocity zone in the upper mantle is a consequence of
580 the steep lithospheric temperature profile within the stagnant lid on Mars (Section 4.1).

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583 **Fig. 6.** Densities of solid (Chen et al., 2008; Komabayashi et al., 2010; Seagle et al., 2006;
 584 Thompson et al., 2016; Urakawa et al., 2004) and liquid (Anderson and Ahrens, 1994; Balog et
 585 al., 2003; Morard et al., 2018; Nishida et al., 2011) alloys in the Fe–S system calculated from
 586 equations of state at 20 GPa and 2000 K. The solid line is a linear fit to the solid data, and the
 587 dashed lines are offset from this line according to fixed ΔV of melting up to the 1 bar ΔV of FeS
 588 (Kaiura and Toguri, 1979). The grey box indicates the range of S contents within uncertainty of
 589 the core formation model and the range of ΔV between that of Fe and FeS at these conditions. All
 590 liquid equations of state have been extrapolated beyond the pressure conditions of the original
 591 measurements, save for the Fe–10S study (Balog et al., 2003) which was based on sink/float
 592 experiments with large ($\sim 20\%$) error bars. Using this data point to derive the properties of the
 593 Fe–S alloy (Khan et al., 2018; Rivoldini et al., 2011) results in an implied ΔV greater than that of
 594 FeS at 1 bar, which is physically unlikely. Red squares represent some previous models of the
 595 Martian core alloy (**a**: Rivoldini et al., 2011; **b**: Khan et al., 2018; **c**: Sohl and Spohn, 1997; **d**:
 596 Zharkov and Gudkova, 2005; **e**: Kavner et al., 2001; **f**: Bertka and Fei, 1998; **g**: Sanloup, 1999;
 597 **h**: Lodders and Fegley, 1997; **i**: Khan and Connolly, 2008). Studies **a–f** are plotted at the same
 598 P – T conditions as the equation of state points, while studies **g–i** have fixed (P – T independent)
 599 core densities.



600

601 **Fig 7.** Tradeoffs between parameters that influence core size as parameterized by Equation 1.

602 Each panel represents a fixed combination of ΔV of melting (constant throughout each column)

603 and mantle potential temperature (constant throughout each row) and shows the combinations of

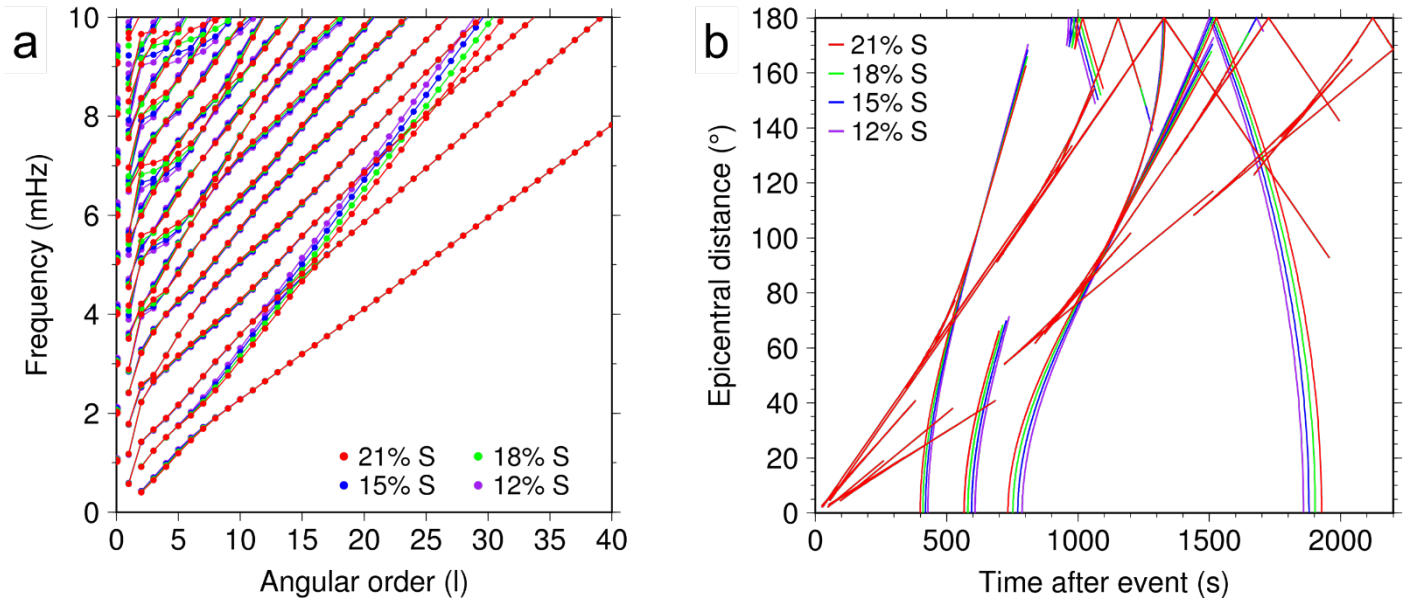
604 core S content and CMB thermal boundary layer temperature contrast that can produce cores of a

605 certain size. Each contour connects cores of the same radius. All plots correspond to a 55 km

606 crust. For this crust size, the approximate MOI constraints on core size (1550–1700 km)

607 are indicated by dashed lines. Supplementary Figure S4 shows alternate versions of this figure

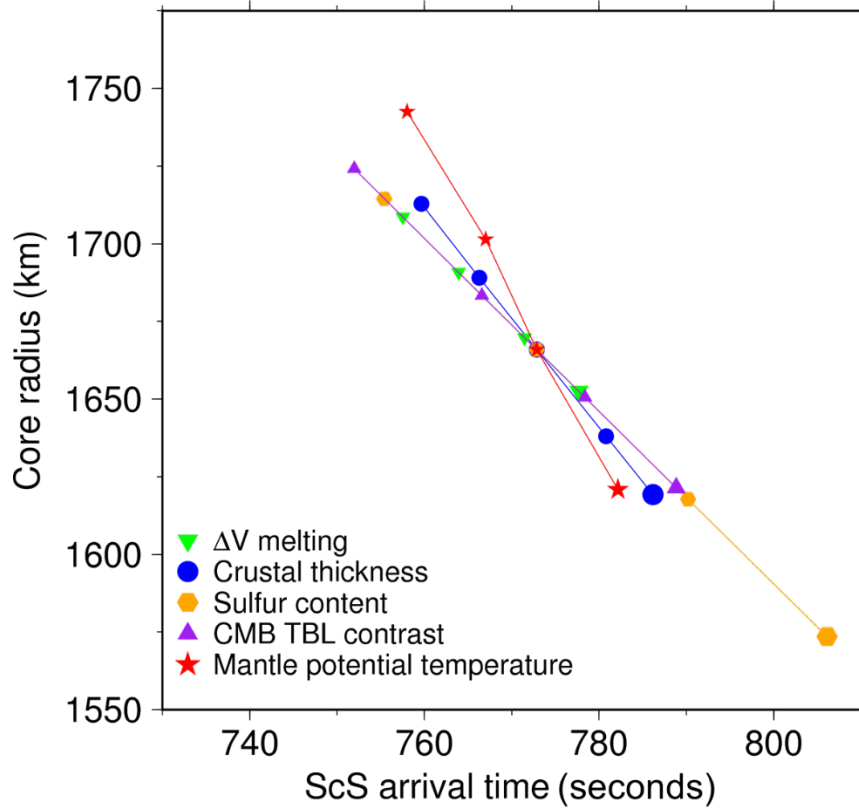
608 corresponding to different crustal thicknesses.



609 **Fig. 8.** Seismological observables corresponding to four models with different core S contents. **a.**
610 Normal mode center frequencies. The radial modes sit on the vertical axis ($l=0$). InSight's
611 broadband seismometer is expected to be unable to detect those modes under 5 mHz. **b.** Body
612 wave travel time predictions for a 5 km deep marsquake. Seismic phases P, PP, PcP, P_{diff}, S, SS,
613 ScS, S_{diff}, PcS, ScP, SP, PKP, SKS, and SKKS are shown.

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617 **Fig. 9.** Relationship between core radius and predicted ScS arrival time. Travel times are
618 predicted for an epicentral distance of 20° and a marsquake depth of 5 km. The impact of each
619 of the five parameters on core radius is discussed in Section 4.4. In each case the larger symbol
620 corresponds to the lowest value of the parameter that is being varied.

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631 **Appendix A. Supplementary materials**

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