



## Supplementary Materials for

### **Curiosity at Gale Crater, Mars: Characterization and Analysis of the Rocknest Sand Shadow**

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## Supplementary Text

### Calculation of mineral compositions from their unit-cell parameters

The chemical compositions of the major mineral phases found in the Rocknest sediment fines were determined by relating their refined unit-cell parameters (Table S1, from (20)) to those published in the literature (22). The figures below show the unit-cell parameter versus chemical composition plots used to estimate the elemental compositions of olivine, plagioclase, augite and pigeonite (Table 3) and their empirical chemical formulas (Table S2).

#### Olivine

The Mg-content of olivine was obtained from the variation of Mg-content versus the unit-cell volume using data from the fayalite-forsterite join (Fig. S1). The least-squares equation for the number of atoms of Mg per formula unit (Mg#) as a function of the unit-cell volume is:

$$\text{Mg\#} = -0.0578V + 17.801$$

#### Plagioclase

The refined unit-cell parameters provided information on the composition of plagioclase feldspar along the Ca-Na join. High-Ca feldspars are characterized by a *c* unit-cell parameter that is double that of lower-Ca feldspars; therefore, our data were restricted to the lower-Ca feldspars. Variations in Ca-content with unit-cell parameters are given in Fig. S2a, S2b and S2c. Fig. S2a shows that the *b* unit-cell parameter is not suitable for determining composition; therefore *c* and *a* were selected to determine the chemistry.

$$\text{Ca\#} = 157.0882779c^2 - 2251.2412721c + 8065.692 \text{ (Fig. S2b)}$$

$$\text{Ca\#} = 0.6896416a^2 - 130.2226916a + 6147.38751 \text{ (Fig. S2c)}$$

#### Augite

Mg-content can be obtained from the variation of the *b* unit-cell parameter (Fig. S3a).

$$\text{Mg\#} = -9.8029b + 88.509$$

Fe/Mg content as a function of  $\beta$  has two sets of well-determined trends, that of  $\text{Ca\#} = 1.0$  and  $\text{Ca\#} = 0.8$  (Fig. S3b). Regressions of Mg-content for these two trends are:

$$\text{Mg\#} = 0.9157\beta - 95.956 \text{ (Ca\# = 1.0)}$$

$$\text{Mg\#} = 1.3719\beta - 144.74 \text{ (Ca\# = 0.8)}$$

Substituting the value of Mg# determined from  $b$  produced  $\beta$  equal to  $105.761^\circ$  for the Ca# = 1.0 trend and  $\beta$  equal to  $106.145^\circ$  for the Ca# = 0.8 trend. Linear interpolation, using our value of  $\beta$ , gives Ca# = 0.75. The value for Fe# = 2 - Mg# - Ca#.

### Pigeonite

The Mg-content of pigeonite can be obtained from the  $b$  unit-cell parameter (Fig. S4a).

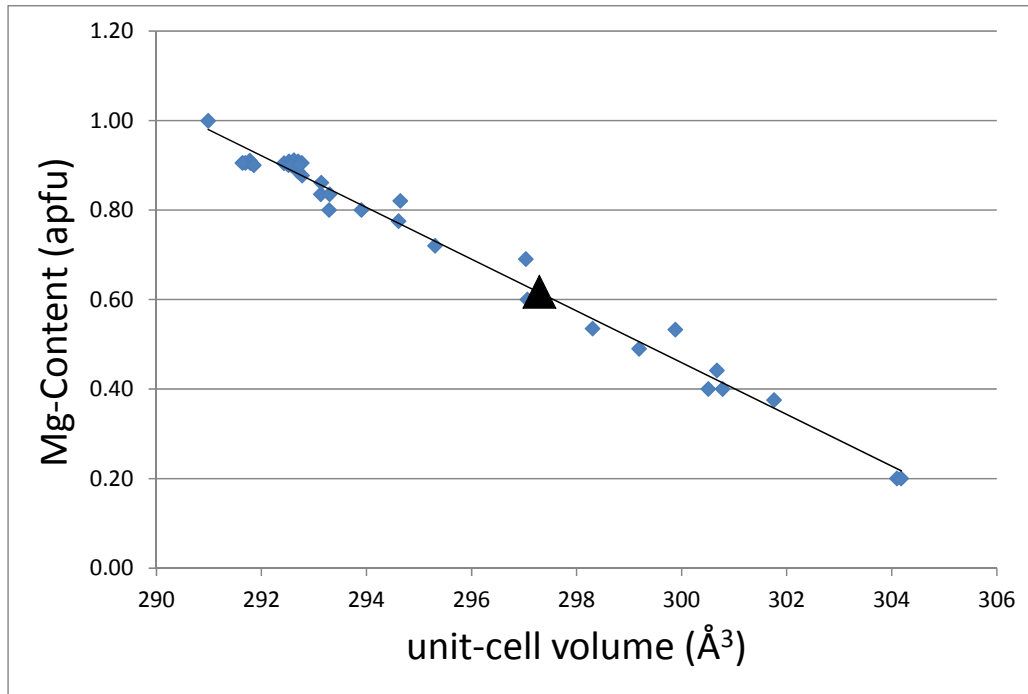
$$\text{Mg\#} = -8.9762b + 81.195$$

The Mg-Ca content as a function of unit-cell volume,  $V$ , has two sets of well-developed trends, that of Fe# = 1 and Fe# = 0 (Fig. S4b). Regressions of Mg-content for these two trends are:

$$\text{Mg\#} = -0.0471V + 21.148 \text{ (Fe\# = 1)}$$

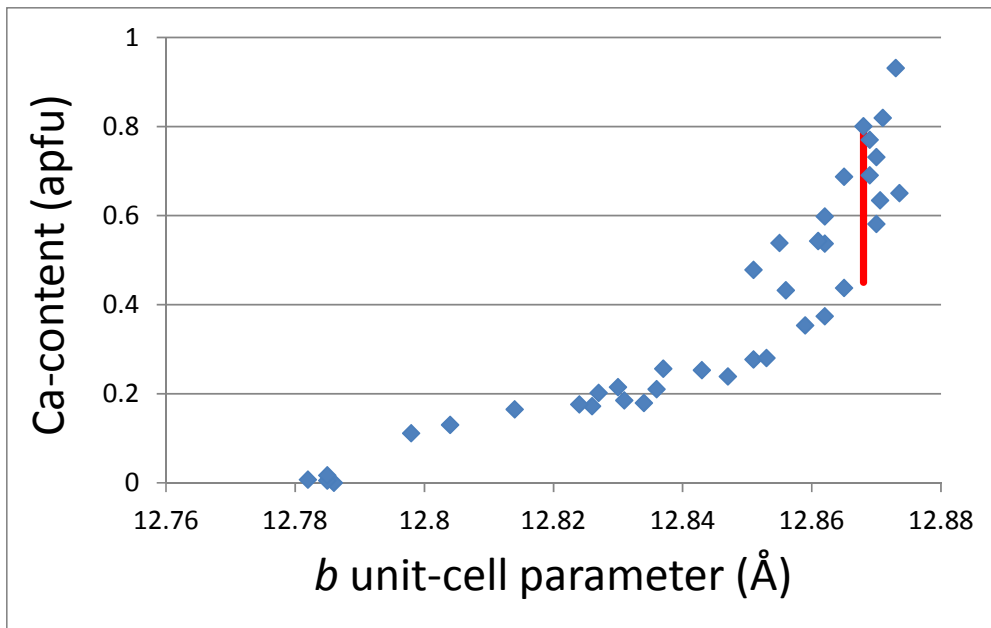
$$\text{Mg\#} = -0.0254V + 12.572 \text{ (Fe\# = 0)}$$

Substituting the refined unit-cell volume from the Rocknest pigeonite gave Mg# = 0.89 for the Fe# = 1 trend and Mg# = 1.65 for the Fe# = 0 trend. Linear interpolation, using the Rocknest pigeonite Mg# estimated from  $b$  (1.13), gives Fe# = 0.68. The values for Ca# = 2 - Mg# - Fe#.



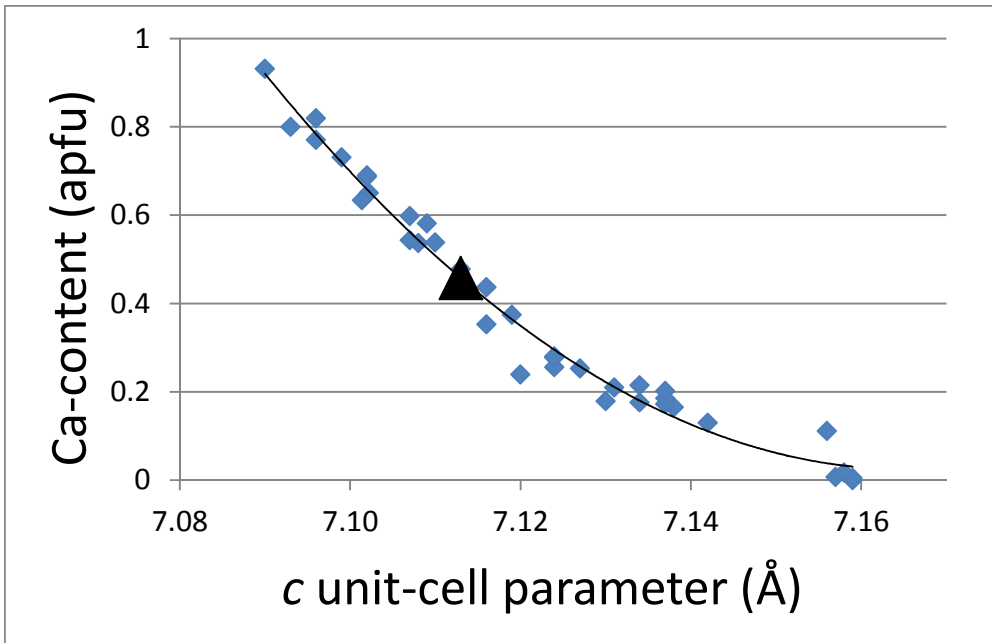
**Fig. S1.**

Mg-content of Fa-Fo olivine as a function of unit-cell volume. The black triangle represents the Rocknest olivine, indicating a composition of Fo 62.



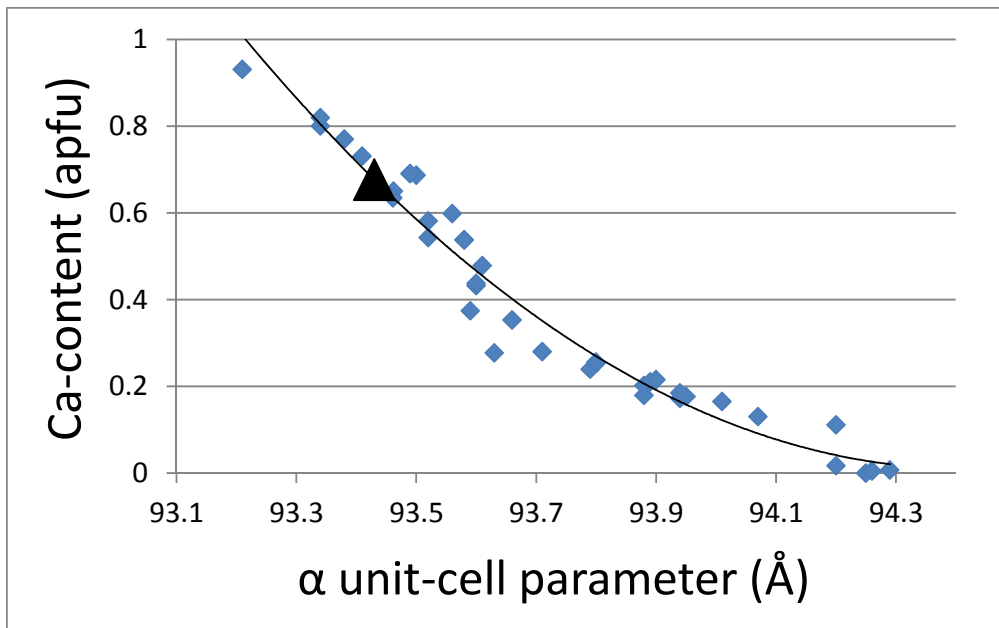
**Fig. S2a**

Ca-content of K-free plagioclase as a function of the *b* unit-cell parameter. The large scatter of data provides an error estimate of 12%.



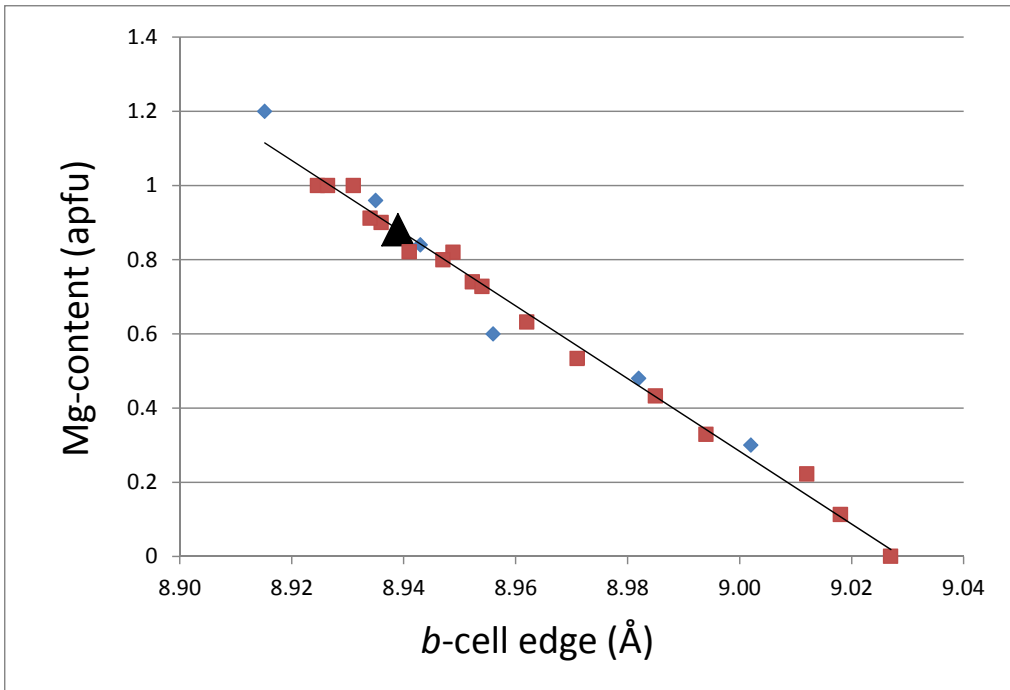
**Fig. S2b**

Ca-content of K-free plagioclase as a function of the  $c$  unit-cell parameter. This trend provides a lower bound on the amount of Ca (black triangle denotes Rocknest data).



**Fig. S2c**

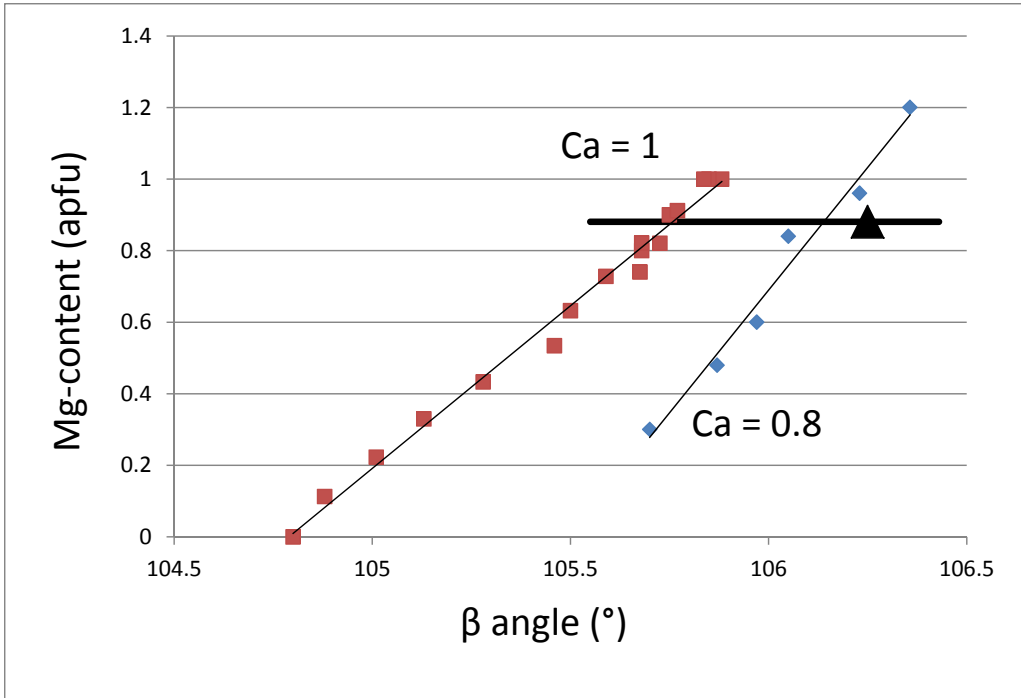
Ca-content of K-free plagioclase as a function of the  $\alpha$  unit-cell parameter. This trend provides an upper bound on the amount of Ca (black triangle represents the Rocknest plagioclase).



**Fig. S3a**

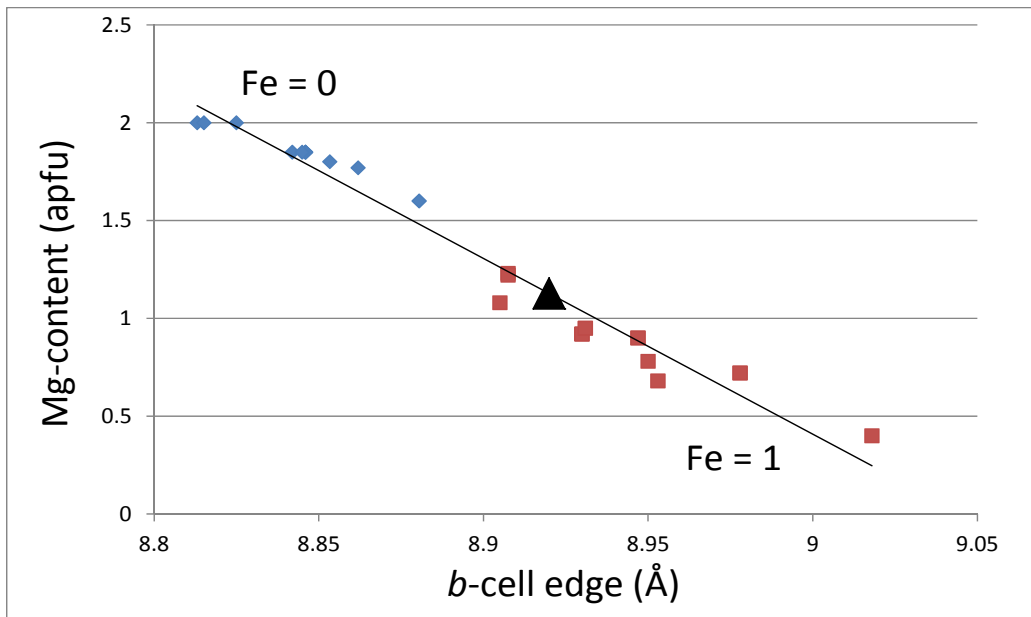
Variation of Mg-content with *b* unit-cell parameter in augite. Blue diamonds represent samples with Ca# = 0.8 and red squares are Ca# = 1. The black triangle represents the Rocknest augite – corresponding to a Mg# of 0.88.





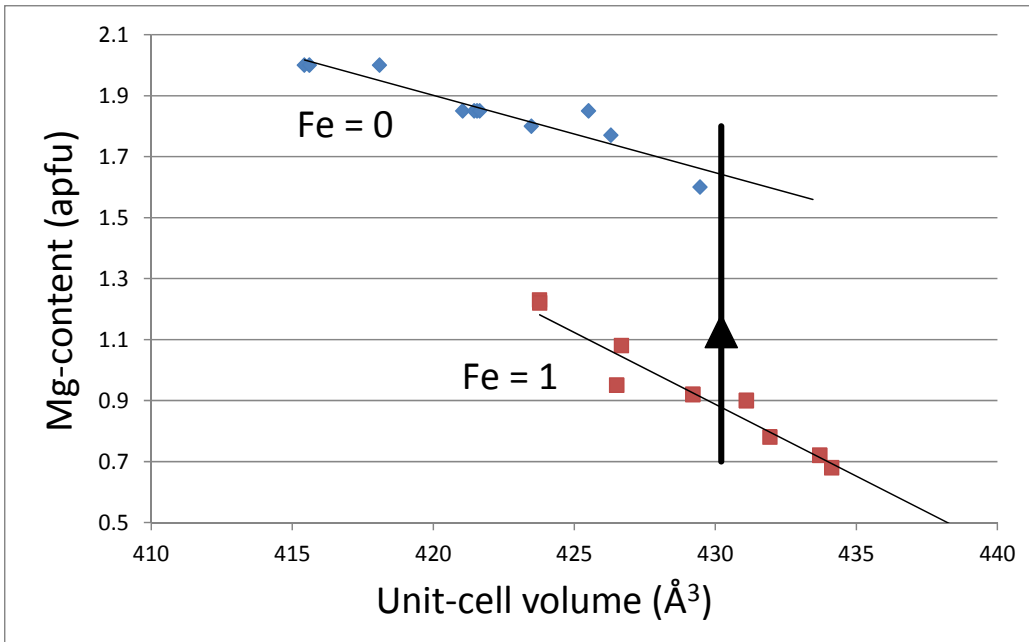
**Fig. S3b**

Ca-content in augite obtained by scaling the separation between the two trends of Mg-content versus  $\beta$  angle at Ca# = 1 (red squares) and Ca# = 0.8 (blue diamonds). The black triangle represents the Rocknest augite Mg-content at the refined  $\beta$  angle and corresponds to Ca# = 0.75.



**Fig. S4a**

Variation of Mg-content with  $b$  unit-cell parameter in pigeonite. Blue diamonds represent  $\text{Fe}\# = 0$  and red squares are  $\text{Fe}\# = 1$ . The estimated  $\text{Mg}\#$  of the Rocknest pigeonite is 1.13 and is marked with the black triangle.



**Fig. S4b**

Fe-content in pigeonite - from the Mg-content determined above and scaling between the trends of samples with no Fe (blue diamonds) and Fe# = 1 (red squares), the Rocknest pigeonite is estimated to contain 0.68 apfu Fe.

**Table S1.**

Wt. % and refined unit-cell parameters of the major crystalline phases in Rocknest (20).

Mineral	Wt.%	2 $\sigma$	$a$ (Å)	$b$ (Å)	$c$ (Å)	$\alpha$ (°)	$\beta$ (°)	$\gamma$ (°)
plagioclase	40.8%	2.4%	8.177(6)	12.868(9)	7.113(5)	93.43(4)	116.26(2)	90.13(3)
forsterite	22.4%	1.9%	10.327(7)	6.034(7)	4.771(5)	90	90	90
augite	14.6%	2.8%	9.782(9)	8.939(9)	5.269(7)	90	106.25(9)	90
pigeonite	13.8%	2.8%	9.652(9)	8.92(1)	5.254(7)	90	108.0(1)	90

**Table S2.**Oxide wt. % compositions of the crystalline mineral phases present in the <150  $\mu\text{m}$  size fraction of Rocknest sediment

	augite	olivine	plagioclase	pigeonite	magnetite	hematite	ilmenite	sanidine	quartz	anhydrite	Total
SiO <sub>2</sub>	53.58	36.49	53.81	53.36	0	0	0	64.76	100	0	48.66
TiO <sub>2</sub>	0	0	0	0	0	0	52.65	0	0	0	0.37
Al <sub>2</sub> O <sub>3</sub>	0	0	29.50	0	0	0	0	18.32	0	0	13.04
FeO	11.85	33.16	0	21.69	87	100	47.35	0	0	0	13.95
MnO	0	0	0	0	0	0	0	0	0	0	0.00
MgO	15.81	30.35	0	20.22	0	0	0	0	0	0	11.17
CaO	18.75	0	11.78	4.73	0	0	0	0	0	41.19	9.30
Na <sub>2</sub> O	0	0	4.91	0	0	0	0	0	0	0	2.11
K <sub>2</sub> O	0	0	0	0	0	0	0	16.92	0	0	0.36
SO <sub>3</sub>	0	0	0	0	0	0	0	0	0	58.81	0.82
Component	0.146	0.224	0.408	0.138	0.021	0.011	0.009	0.013	0.014	0.015	

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31. Because APXS does not discriminate among iron oxidation states, the total Fe concentration was proportioned in accordance with the oxidation state information carried by the crystalline phases (Table 3, column 3). FeO-Cryst and Fe<sub>2</sub>O<sub>3</sub>-Cryst are the concentrations of FeO and Fe<sub>2</sub>O<sub>3</sub> required to accommodate olivine, augite, pigeonite, ilmenite, and magnetite and hematite, in accordance with their valence states. The remaining iron (FeO + Fe<sub>2</sub>O<sub>3</sub>) is then associated with the amorphous component without implications for oxidation state. Similarly, some SO<sub>3</sub> is reported as SO<sub>3</sub>-Cryst to accommodate anhydrite as a crystalline component.
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33. Nanophase ferric oxide (npOx) is a generic name for amorphous, poorly crystalline, or short-range ordered products of oxidative alteration/weathering that have octahedrally coordinated Fe<sup>3+</sup> (Mössbauer doublet) and are predominantly oxide/oxyhydroxide/hydrous in nature. Depending on local conditions, npOx (as encountered on Earth) can be any combination of superparamagnetic hematite and goethite, lepidocrocite, ferrihydrite, schwertmannite, akaganeite, hisingerite, and the octahedral Fe<sup>3+</sup>-rich particles that pigment iddingsite and palagonite. npOx can also incorporate anions like (SO<sub>4</sub>)<sup>2-</sup>, Cl<sup>-</sup>, and (PO<sub>4</sub>)<sup>3-</sup> through specific chemical adsorption. Because of different local conditions on Mars, one or more forms of npOx on the planet may be uncommon or not present on Earth.
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