Supplementary Material

The solubility of molecular hydrogen in silicate melts and the origin of hydrogen in the interiors of terrestrial planets

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Contributions to Mineralogy and Petrology

This supplementary material contains Table S1 with the data for the magma ocean – primordial atmosphere model presented in Figure 10 of the main article.

Table S1 Model of a primordial H_2-H_2O atmosphere as a function of oxygen fugacity

$log f_{O_2}$	P^{total}	H_2/H_2O	P_{H_2}	P_{H_2O}	$c^{melt}_{H_2}$	$c^{melt}_{H_2O}$	$m^{melt}_{H_2}$	$m^{melt}_{H_2O}$	$m^{atmosphere}$	$m^{gas}_{H_2}$	$m^{gas}_{H_2O}$	$m^{total}_{H_2O}$
ΔIW	MPa		MPa	MPa	ppm	wt.%	as kg H_2O	kg	kg	as kg H_2O	kg	as kg H_2O
0	98.2	0.86	45.3	52.9	23.3	2.31	$8.490 \cdot 10^{20}$	$9.339 \cdot 10^{22}$	$5.100 \cdot 10^{21}$	$3.989 \cdot 10^{21}$	$4.658 \cdot 10^{21}$	$1.0289 \cdot 10^{23}$
-0.25	108.5	1.14	57.8	50.7	29.8	2.25	$1.084 \cdot 10^{21}$	$9.109 \cdot 10^{22}$	$5.640 \cdot 10^{21}$	$5.711 \cdot 10^{21}$	$5.001 \cdot 10^{21}$	$1.0289 \cdot 10^{23}$
-0.5	120.4	1.52	72.7	47.7	37.4	2.18	$1.362 \cdot 10^{21}$	$8.803 \cdot 10^{22}$	$6.255 \cdot 10^{21}$	$8.148 \cdot 10^{21}$	$5.350 . 10^{21}$	$1.0289 \cdot 10^{23}$
-0.75	133.5	2.03	89.5	44.1	46.1	2.08	$1.677 \cdot 10^{21}$	$8.406 \cdot 10^{22}$	$6.936 \cdot 10^{21}$	$1.149 \cdot 10^{22}$	$5.659 . 10^{21}$	$1.0289 \cdot 10^{23}$
-1	147.0	2.71	107.4	39.6	55.3	1.96	$2.012 \cdot 10^{21}$	$7.911 \cdot 10^{22}$	$7.637 \cdot 10^{21}$	$1.590 \cdot 10^{22}$	$5.870 \cdot 10^{21}$	$1.0289 \cdot 10^{23}$
-1.25	159.9	3.61	125.2	34.7	64.5	1.81	$2.346 \cdot 10^{21}$	$7.322 . 10^{22}$	$8.303 \cdot 10^{21}$	$2.140 \cdot 10^{22}$	$5.925 \cdot 10^{21}$	$1.0289 \cdot 10^{23}$
-1.5	171.0	4.82	141.6	29.4	72.9	1.65	$2.653 \cdot 10^{21}$	$6.659 \cdot 10^{22}$	$8.881 \cdot 10^{21}$	$2.786 \cdot 10^{22}$	$5.785 \cdot 10^{21}$	$1.0289 \cdot 10^{23}$
-1.75	179.7	6.42	155.5	24.2	80.1	1.47	$2.914 \cdot 10^{21}$	$5.955 \cdot 10^{22}$	$9.334 \cdot 10^{21}$	$3.498 \cdot 10^{22}$	$5.447 \cdot 10^{21}$	$1.0289 \cdot 10^{23}$
-2	185.8	8.56	166.4	19.4	85.7	1.30	$3.118 \cdot 10^{21}$	$5.246 \cdot 10^{22}$	$9.653 \cdot 10^{21}$	$4.236 \cdot 10^{22}$	$4.946 \cdot 10^{21}$	$1.0289 \cdot 10^{23}$
-2.25	189.7	11.42	174.4	15.3	89.8	1.13	$3.269 \cdot 10^{21}$	$4.568 \cdot 10^{22}$	$9.854 \cdot 10^{21}$	$4.960 \cdot 10^{22}$	$4.343 \cdot 10^{21}$	$1.0289 \cdot 10^{23}$
-2.5	191.9	15.23	180.1	11.8	92.8	0.97	$3.375 \cdot 10^{21}$	$3.942 \cdot 10^{22}$	$9.969 \cdot 10^{21}$	$5.639 \cdot 10^{22}$	$3.703 \cdot 10^{21}$	$1.0289 \cdot 10^{23}$
-2.75	193.1	20.31	184.0	9.06	94.8	0.84	$3.449 \cdot 10^{21}$	$3.381 \cdot 10^{22}$	$1.003 \cdot 10^{22}$	$6.255 \cdot 10^{22}$	$3.080 \cdot 10^{21}$	$1.0289 \cdot 10^{23}$
-3	193.7	27.08	186.8	6.90	96.2	0.71	$3.501 \cdot 10^{21}$	$2.890 \cdot 10^{22}$	$1.006 \cdot 10^{22}$	$6.798 \cdot 10^{22}$	$2.510 \cdot 10^{21}$	$1.0289 \cdot 10^{23}$
-3.25	194.2	36.12	189.	5.23	97.3	0.61	$3.542 \cdot 10^{21}$	$2.465 \cdot 10^{22}$	$1.009 \cdot 10^{22}$	$7.269 \cdot 10^{22}$	$2.013 \cdot 10^{21}$	$1.0289 \cdot 10^{23}$
-3.5	194.8	48.16	190.8	3.96	98.3	0.52	$3.576 \cdot 10^{21}$	$2.100 \cdot 10^{22}$	$1.012 \cdot 10^{22}$	$7.672 \cdot 10^{22}$	$1.593 \cdot 10^{21}$	$1.0289 \cdot 10^{23}$
-3.75	195.5	64.22	192.4	3.00	99.1	0.44	$3.607 \cdot 10^{21}$	$1.788 \cdot 10^{22}$	$1.015 \cdot 10^{22}$	$8.015 \cdot 10^{22}$	$1.248 \cdot 10^{21}$	$1.0289 \cdot 10^{23}$
-4	196.3	85.64	194.1	2.27	100.0	0.38	$3.637 \cdot 10^{21}$	$1.522 . 10^{22}$	$1.020 \cdot 10^{22}$	$8.306 \cdot 10^{22}$	$9.698 \cdot 10^{20}$	$1.0289 \cdot 10^{23}$
-4.25	197.4	114.2	195.6	1.71	100.8	0.32	$3.666 \cdot 10^{21}$	$1.296 \cdot 10^{22}$	$1.025 \cdot 10^{22}$	$8.552 \cdot 10^{22}$	$7.488 \cdot 10^{20}$	$1.0289 \cdot 10^{23}$
-4.5	198.4	152.3	197.2	1.29	101.5	0.27	$3.694 \cdot 10^{21}$	$1.103 \cdot 10^{22}$	$1.031 \cdot 10^{22}$	$8.759 \cdot 10^{22}$	$5.751 \cdot 10^{20}$	$1.0289 \cdot 10^{23}$
-4.75	199.6	203.1	198.6	0.98	102.3	0.23	$3.722 \cdot 10^{21}$	$9.384 \cdot 10^{21}$	$1.037 \cdot 10^{22}$	$8.934 \cdot 10^{22}$	$4.399 \cdot 10^{20}$	$1.0289 \cdot 10^{23}$
-5	200.7	270.8	200.0	0.74	103.0	0.20	$3.748 \cdot 10^{21}$	$7.983 \cdot 10^{21}$	$1.043 \cdot 10^{22}$	$9.082 \cdot 10^{22}$	$3.354 \cdot 10^{20}$	$1.0289 \cdot 10^{23}$
-5.25	201.9	361.2	201.3	0.56	103.7	0.17	$3.772 \cdot 10^{21}$	$6.789 \cdot 10^{21}$	$1.049 \cdot 10^{22}$	$9.207 \cdot 10^{22}$	$2.549 \cdot 10^{20}$	$1.0289 \cdot 10^{23}$
-5.5	203.0	491.6	202.6	0.41	104.3	0.14	$3.797 \cdot 10^{21}$	$5.705 \cdot 10^{21}$	$1.054 \cdot 10^{22}$	$9.320 \cdot 10^{22}$	$1.896 \cdot 10^{20}$	$1.0289 \cdot 10^{23}$
-5.75	203.9	642.2	203.6	0.32	104.9	0.12	$3.816 \cdot 10^{21}$	$4.906 \cdot 10^{21}$	$1.059 \cdot 10^{22}$	$9.402 \cdot 10^{22}$	$1.464 \cdot 10^{20}$	$1.0289 \cdot 10^{23}$
-6	204.9	856.4	204.6	0.24	105.4	0.10	$3.835 \cdot 10^{21}$	$4.168 \cdot 10^{21}$	$1.064 \cdot 10^{22}$	$9.478 \cdot 10^{22}$	$1.107 \cdot 10^{20}$	$1.0289 \cdot 10^{23}$

Notes:

$log f_{O_2}$ is the logarithm of the oxygen fugacity relative to the Fe-FeO buffer (ΔIW)

P^{total} is the total gas pressure of the atmosphere in MPa. To achieve mass balance, this value was adjusted by hand until the total mass of hydrogen (expressed as kg H_2O) in the system (last column) reached the desired value of $1.0289 \cdot 10^{23}$

H_2/H_2O is the molar ratio of H_2 to H_2O in the gas phase, calculated from the equilibrium $H_2 + ½ O_2 = H_2O$, using the oxygen fugacity given in the first column of the table

P_{H_2} is the partial pressure of hydrogen in the atmosphere in MPa. It is calculated from the total pressure in the second column and the H_2/H_2O ratio in the third column.

P_{H_2O} is the partial pressure of H_2O in the atmosphere in MPa. It is calculated from the total pressure in the second column and the H_2/H_2O ratio in the third column.

$c_{H_2}^{melt}$ is the concentration of H_2 in the melt (expressed as ppm by weight, μg/g). This is calculated from P_{H_2} assuming a solubility (see main text) of 515 ppm H_2 per GPa H_2 partial pressure.

$c_{H_2O}^{melt}$ is the concentration of H_2O in the melt in wt. %. This is calculated from P_{H_2O} using the solubility law for water in basaltic melt by Shishkina et al. (2010)

$m_{H_2}^{melt}$ is the mass of H_2 dissolved in the melt (magma ocean), but expressed as the equivalent mass of H_2O in kg

$m_{H_2O}^{melt}$ is the mass of H_2O dissolved in the melt (magma ocean) in kg

$m^{atmophere}$ is the mass of the atmosphere in kg, as calculated from the total atmospheric pressure in the second column

$m_{H_2}^{gas}$ is the mass of H_2 in the atmosphere, but expressed as the equivalent mass of H_2O in kg

$m_{H_2O}^{gas}$ is the mass of H_2O in the atmosphere in kg

$m_{H_2O}^{total}$ is the total mass of H_2 and H_2O in both melt (magma ocean) and gas (primordial atmosphere) combined, all expressed as kg H_2O. The total atmospheric pressure in column 2 was for every oxygen fugacity adjusted by hand such that $m_{H_2O}^{total}$ yielded a value of $1.0289 \cdot 10^{23}$kg. This is the mass of hydrogen (expressed as kg H_2O) in a planet with the mass of the current Earth, made of 95 % ordinary chondrite material and 5 % of CI chondrite. See the main text for further details.