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SUPPLEMENTARY MATERIAL TO

A multidisciplinary study on magnesium

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SUPPLEMENT A

Astrophysics, geophysics, geochemistry

The Earth is built by three major and distinctly different units: the core, the mantle-crust system (silicate Earth) and the atmosphere–hydrosphere system, being the products of planetary differentiation and having very different composition.[1,2] While the composition of the crust and the atmosphere–hydrosphere system can be determined by usual experimental methods, information about the Earth's mantel and, particularly, core has been gathered more or less indirectly. One of the key tools thereby is the (logical) assumption, partly verified by measurements, that the global composition of the Earth cannot be much different from that of the other objects with the common origin, *i.e.*, of those belonging to the Solar system. The most easily accessible objects of such an art are meteorids, because around 15,000 tonnes of them enter the Earth's atmosphere each year. (One should make distinction between "meteorid", "meteor", and "meteorite". Meteoroids are sand- to boulder-sized particles of debris in the Solar system. The visible path of a meteoroid (when it begins to heat up and break apart) that enters the Earth's atmosphere is called a meteor. If a meteoroid reaches the ground and survives impact, then it is called a meteorite). There are several types of meteorids/meteorites, including stony, carbonaceous chondrites and iron–nickel ones. Magnesium is an important constituent of a number of meteorid types.

The investigations on the Earth's composition have lead to the following conclusions. The radius of the core is about 1/2 that of the Earth's, and thus its volume is about 1/8 of the Earth's. However, the mass of the core is roughly 1/3 of the Earth's mass, because the core is about 90 % of an Fe–Ni (heavy-metal)

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alloy (with a dominating contribution of iron, 85 % against 5 % Ni). The main constituents of the mantle and crust are silicates containing primarily magnesium, iron, aluminium and calcium. The most abundant element in this part of the Earth is O (44 %), followed by Mg (22.8 %), Si (21 %), Fe (6.3 %), and Al (2.35 %).[1]

Beside being an important constituent of the Earth, Mg has been used for dating of different astrophysical and geological events and processes. It has three stable isotopes: ^{24}Mg, ^{25}Mg and ^{26}Mg. All are present in significant amounts. About 79 % of Mg is ^{24}Mg. ^{24}Mg is produced in stars larger than 3 solar masses by fusing helium and neon in the alpha process at temperatures above 600 mega-kelvins. Its large abundance in the universe (it is believed to be the ninth most frequent element) is connected with the fact that its nucleus is a multiple of an *α* particle. ^{26}Mg has found application in isotopic geology as a radiogenic daughter product of ^{26}Al, which has a half-life of 717,000 years.[3]

SUPPLEMENT B

TABLE S-I. A part of the table with molecular constants for ^{24}Mg^{16}O given by HH[4]

State	T_e / cm^{-1}	ω_e / cm^{-1}	$\omega_e x_e$ / cm^{-1}	r_e / Å	Observed transitions	ν_{00} / cm^{-1}
$G\ ^1\Pi$	[40259.8]	–	–	[1.834]	$G \rightarrow A$	36365.$_4$
					$G \rightarrow X$	39868.$_6$
$F\ ^1\Pi$	(37922)	[696]	–	[1.772$_8$]	$F \rightarrow X$	37879.1
$E\ ^1\Sigma^+$	(37722)	[705]	–	[1.829]	$E \rightarrow A$	34180
					$E \rightarrow X$	37683.$_5$
$C\ ^1\Sigma^-$	30080.6	632.4	5.2	[1.872$_9$]	$C \rightarrow A$	26500.94
$e\ ^3\Sigma^-$	–	–	–	–	$(e \leftarrow a)$	–
$D\ ^1\Delta$	29851.6	632.5	5.3	1.871$_8$	$D \rightarrow A$	26272.04
$d\ ^3\Delta_i$	(29300)	(650)		(1.8$_7$)	$(d \leftrightarrow a)$	26867
$c\ ^3\Sigma^+$	(28300)				$(c \leftarrow a)$	25900
$B\ ^1\Sigma^+$	19984.0	824.0$_8$	4.7$_6$	1.737$_1$	$B \rightarrow A$	16500.2$_9$
					$B \rightarrow X$	20003.5$_7$
$A\ ^1\Pi$	3563.3	664.4$_4$	3.91	1.864$_0$	–	–
$a\ ^3\Pi_i$	(2400)	(650)		(1.8$_7$)	–	–
$X\ ^1\Sigma^+$	0	785.0$_6$	5.1$_8$	1.749$_0$	–	–

SUPPLEMENT C

Perturbative treatment of a one-dimensional anharmonic oscillator

In the perturbative and variation approaches to the Schrödinger equation of an one-dimensional anharmonic oscillator, used in the present study, the matrix elements ξ, ξ^2, ξ^3 and ξ^4 in the basis consisting of eigenfunctions, Eq. (12) in the parent paper. The only non-vanishing matrix elements are:

$$\langle \mathrm{v}+1 | \xi | \mathrm{v} \rangle = \sqrt{\frac{\mathrm{v}+1}{2}} \tag{C.1}$$

$$\langle \mathrm{v}|\xi^2|\mathrm{v}\rangle = \left(\mathrm{v}+\frac{1}{2}\right),\quad \langle \mathrm{v}+2|\xi^2|\mathrm{v}\rangle = \frac{\sqrt{(\mathrm{v}+1)(\mathrm{v}+2)}}{2} \tag{C.2}$$

$$\langle \mathrm{v}+1|\xi^3|\mathrm{v}\rangle = \frac{3\sqrt{(\mathrm{v}+1)^3}}{\sqrt{8}},\quad \langle \mathrm{v}+3|\xi^3|\mathrm{v}\rangle = \frac{\sqrt{(\mathrm{v}+1)(\mathrm{v}+2)(\mathrm{v}+3)}}{\sqrt{8}} \tag{C.3}$$

and

$$\langle \mathrm{v}|\xi^4|\mathrm{v}\rangle = \frac{3}{4}\left(2\mathrm{v}^2+2\mathrm{v}+1\right),\quad \langle \mathrm{v}+2|\xi^4|\mathrm{v}\rangle = \left(\mathrm{v}+\frac{3}{2}\right)\sqrt{(\mathrm{v}+2)(\mathrm{v}+1)},$$
$$\langle \mathrm{v}+4|\xi^4|\mathrm{v}\rangle = \frac{\sqrt{(\mathrm{v}+4)(\mathrm{v}+3)(\mathrm{v}+2)(\mathrm{v}+1)}}{4} \tag{C.4}$$

Applying the Rayleigh–Schrödinger perturbative approach, one obtains for the energy up to fourth order the formulae:

$$E_\mathrm{v}^{(1)} = \left\langle \psi_\mathrm{v}^{(0)} \middle| V' \middle| \psi_\mathrm{v}^{(0)} \right\rangle \equiv V'_{\mathrm{vv}},$$

$$E_\mathrm{v}^{(2)} = \sum_{i\neq \mathrm{v}} \frac{|V'_{i\mathrm{v}}|^2}{E_\mathrm{v}^{(0)} - E_i^{(0)}}, \tag{C.5}$$

$$E_\mathrm{v}^{(3)} = \sum_{i\neq \mathrm{v}}\sum_{k\neq \mathrm{v}} \frac{V'_{\mathrm{v}i}V'_{ik}V'_{k\mathrm{v}}}{\left(E_\mathrm{v}^{(0)}-E_i^{(0)}\right)\left(E_\mathrm{v}^{(0)}-E_k^{(0)}\right)} - V'_{\mathrm{vv}}\sum_{i\neq \mathrm{v}} \frac{|V'_{i\mathrm{v}}|^2}{\left(E_\mathrm{v}^{(0)}-E_i^{(0)}\right)},$$

and

$$E_\mathrm{v}^{(4)} = \sum_{i\neq \mathrm{v}}\sum_{j\neq \mathrm{v}}\sum_{k\neq \mathrm{v}} \frac{V_{\mathrm{v}i}^{(1)}V_{ij}^{(1)}V_{jk}^{(1)}V_{k\mathrm{v}}^{(1)}}{\left[E_\mathrm{v}^{(0)}-E_i^{(0)}\right]\left[E_\mathrm{v}^{(0)}-E_j^{(0)}\right]\left[E_\mathrm{v}^{(0)}-E_k^{(0)}\right]} -$$
$$-2V_{\mathrm{vv}}^{(1)}\sum_{i\neq \mathrm{v}}\sum_{k\neq \mathrm{v}} \frac{V_{\mathrm{v}i}^{(1)}V_{ik}^{(1)}V_{k\mathrm{v}}^{(1)}}{\left[E_\mathrm{v}^{(0)}-E_i^{(0)}\right]^2\left[E_\mathrm{v}^{(0)}-E_k^{(0)}\right]} + \tag{C.6}$$
$$+\left[V_{\mathrm{vv}}^{(1)}\right]^2\sum_{i\neq \mathrm{v}} \frac{\left|V_{i\mathrm{v}}^{(1)}\right|^2}{\left[E_\mathrm{v}^{(0)}-E_i^{(0)}\right]^3} - \sum_{i\neq \mathrm{v}}\sum_{k\neq \mathrm{v}} \frac{\left|V_{i\mathrm{v}}^{(1)}\right|^2\left|V_{k\mathrm{v}}^{(1)}\right|^2}{\left[E_\mathrm{v}^{(0)}-E_i^{(0)}\right]\left[E_\mathrm{v}^{(0)}-E_k^{(0)}\right]^2}$$

where:

$$V'_{i\mathrm{v}} \equiv \left\langle \psi_i^{(0)} \middle| V' \middle| \psi_{\mathrm{v}}^{(0)} \right\rangle \tag{C.7}$$

In the case of a one-dimensional anharmonic oscillator, the cubic term in Eq. (35) from the parent paper, involving ξ^3, does not contribute to the first- and the third-order energy correction. The fourth-order energy contribution of this term is,

$$E_{\mathrm{v},3}^{(4)} = \sum_{i\neq \mathrm{v}} \sum_{j\neq \mathrm{v}} \sum_{k\neq \mathrm{v}} \frac{V_{\mathrm{v}i}^{(1)} V_{ij}^{(1)} V_{jk}^{(1)} V_{k\mathrm{v}}^{(1)}}{\left[E_{\mathrm{v}}^{(0)} - E_i^{(0)}\right]\left[E_{\mathrm{v}}^{(0)} - E_j^{(0)}\right]\left[E_{\mathrm{v}}^{(0)} - E_k^{(0)}\right]} - -E_{\mathrm{v}}^{(2)} \sum_{j\neq \mathrm{v}} \frac{\left|V_{j\mathrm{v}}^{(1)}\right|^2}{\left[E_{\mathrm{v}}^{(0)} - E_j^{(0)}\right]^2} \tag{C.8}$$

Using the above presented expressions, one obtains the formulae (40–42) in the parent paper.

SUPPLEMENT D

Details of the method for the calculation of the plasma composition

We start with any positive set of values $X^{(0)} = \{x_1^{(0)}, x_2^{(0)},\ldots, x_n^{(0)}\}$ that satisfies the conditions (62) and forms an expression analogous to Eq. (59) in the parent paper:

$$G\left[X^{(0)}\right] = \sum_{i=1}^{n} x_i^{(0)} \left[c_i + \ln \frac{x_i^{(0)}}{\overline{x}^{(0)}}\right] \tag{D.1}$$

with:

$$\overline{x}^{(0)} = \sum_{i=1}^{n} x_i^{(0)} \tag{D.2}$$

Of course, (S.1) will be a poor approximation to Eq. (59) from the parent paper. Thus, now a new set of coefficients, $X^{(1)} = \{x_1^{(1)}, x_2^{(1)}, \ldots x_n^{(1)}\}$, must be searched for that gives the function:

$$G\left[X^{(1)}\right] = \sum_{i=1}^{n} x_i^{(1)} \left[c_i + \ln \frac{x_i^{(1)}}{\overline{x}^{(1)}}\right] \tag{D.3}$$

with

$$\bar{x}^{(1)} = \sum_{i=1}^{n} x_i^{(1)} \qquad \text{(D.4)}$$

to be a better approximation to Eq. (59) in the parent paper. Let $\Delta_i \equiv x_i^{(1)} - x_i^{(0)}$ and $\bar{\Delta} = \bar{x}_i^{(1)} - x^{(0)}$. We expand the function $G\left|X^{(1)}\right|$ assuming $X^{(1)} = \{x_1^{(1)}, x_2^{(1)},\dots, x_n^{(1)}\}$, to be variables in a second-order Taylor series about $X^{(0)}$:

$$\begin{aligned}
Q\left[X^{(1)}\right] &= \left\{G\left[X^{(1)}\right]\right\}_{X^{(1)}=X^{(0)}} + \sum_{i=1}^{n}\left\{\frac{\partial G\left[X^{(1)}\right]}{\partial x_i^{(0)}}\right\}_{X^{(1)}=X^{(0)}} \Delta_i + \\
&+ \frac{1}{2}\sum_{i=1}^{n}\sum_{k=1}^{n}\left\{\frac{\partial^2 G\left[X^{(1)}\right]}{\partial x_i^{(0)}\partial x_i^{(0)}}\right\}_{X^{(1)}=X^{(0)}} \Delta_i\Delta_k = \\
&= G\left[X^{(0)}\right] + \sum_{i=1}^{n}\left[c_i + \ln\frac{x_i^{(0)}}{\bar{x}^{(0)}}\right]\Delta_i + \frac{1}{2}\sum_{i=1}^{n}\Delta_i\left[\frac{\Delta_i}{x_i^{(0)}} - \frac{\bar{\Delta}}{\bar{x}^{(0)}}\right] = \qquad \text{(D.5)}\\
&\equiv G\left[X^{(0)}\right] + \sum_{i=1}^{n}\left[c_i + \ln\frac{x_i^{(0)}}{\bar{x}^{(0)}}\right]\left[x_i^{(1)} - x_i^{(0)}\right] + \\
&+ \frac{1}{2}\sum_{i=1}^{n}\left[x_i^{(1)} - x_i^{(0)}\right]\left[\frac{x_i^{(1)} - x_i^{(0)}}{x_i^{(0)}} - \frac{\bar{x}^{(1)} - \bar{x}^{(0)}}{\bar{x}^{(0)}}\right].
\end{aligned}$$

(This equation (in a somewhat different notation) is erroneously typed in the original paper.[70])

Knowing that the optimal coefficients $X = \{x_1, x_2, \dots x_n\}$ lead to the condition $\partial G(X) / \partial x_i = 0$ for all x_i, the derivatives of the function $Q\left|X^{(1)}\right|$ are set to zero. However, this cannot be done directly because the variables $X^{(1)} = \{x_1^{(1)}, x_2^{(1)},\dots, x_n^{(1)}\}$ [unlike the zero-th-order coefficients $X^{(0)} = \{x_1^{(0)}, x_2^{(0)},\dots, x_n^{(0)}\}$] do not automatically satisfy the conditions (62) in the parent paper. Thus, the fulfilment of these conditions must be ensured. This can be realised by applying the method of Lagrange multipliers. The function $Q\left|X^{(1)}\right|$ is replaced by:

$$H\left[X^{(1)}\right] = Q\left[X^{(1)}\right] - \sum_{k=1}^{m+1}\pi_k\left[a_{ik}x_i^{(1)} - b_k\right] \qquad \text{(D.6)}$$

where π_k are yet undetermined Lagrange multipliers. The conditions $\partial H\left|X^{(1)}\right| / \partial x_i^{(0)} = 0$ lead to a set of equations:

$$\frac{\partial H\left[X^{(1)}\right]}{\partial x_i^{(1)}}=\left[c_i+\ln\frac{x_i^{(0)}}{\overline{x}^{(0)}}\right]+\left[\frac{x_i^{(1)}}{x_i^{(0)}}-\frac{\overline{x}^{(1)}}{\overline{x}^{(0)}}\right]-\sum_{k=1}^{m+1}\pi_k a_{ik}=0, \tag{D.7}$$

$$i=1,\ 2,\dots,\ n$$

Equation (D.7) and:

$$\sum_{k=1}^{n}x_i^{(1)}a_{ik}=b_k\,,\quad k=1,\ 2,\dots,\ m+1 \tag{D.8}$$

represent (when $\overline{x}^{(1)}$ is substituted by the right-hand side of Eq. (D.4)) a system of $n+m+1$ linear equations, the solutions of which are the new generation of coefficients, $X^{(1)} = \{x_1^{(1)}, x_2^{(1)},\dots, x_n^{(1)}\}$, and the Lagrange multipliers $\pi_1, \pi_2,\dots, \pi_{m+1}$. The coefficients $X^{(1)} = \{x_1^{(1)}, x_2^{(1)},\dots, x_n^{(1)}\}$ are employed to obtain (D.3). A new function:

$$G\left[X^{(2)}\right]=\sum_{i=1}^{n}x_i^{(2)}\left[c_i+\ln\frac{x_i^{(2)}}{\overline{x}^{(2)}}\right] \tag{D.9}$$

is supposed, where now the new coefficients $X^{(2)} = \{x_1^{(2)}, x_2^{(2)},\dots, x_n^{(2)}\}$ are handled as variables, and this function is expanded in a Taylor series about $X^{(1)}$. The procedure is repeated until convergence is achieved.

It was shown[80] that the mathematical problem can be reduced to the solution of a system of $m + 2$ (*i.e.*, in the original work to $m + 1$, because White *et al*. did not consider the constraint (61) in the parent paper) equations. Thus, the size of the system of linear equations to be solved can be reduced (practically) to the number of elements in question. From Eq. (D.7), it follows, namely:

$$x_i^{(1)}=-x_i^{(0)}f_i\left[X^{(0)}\right]+\frac{x_i^{(0)}}{\overline{x}^{(0)}}\overline{x}^{(1)}+x_i^{(0)}\sum_{k=1}^{m+1}\pi_k a_{ik} \tag{D.10}$$

where:

$$f_i\left[X^{(0)}\right]\equiv\left[c_i+\ln\frac{x_i^{(0)}}{\overline{x}^{(0)}}\right] \tag{D.11}$$

Summing over i in Eq. (D.11), when Eq. (62) from the parent paper is taken into account, gives:

$$\sum_{k=1}^{m+1}\pi_k b_k=\sum_{i=1}^{n}x_i^{(0)}f_i\left[X^{(0)}\right] \tag{D.12}$$

Inserting Eq. (D.10) into Eq. (D.8), and using the condition (62) from the parent paper, one obtains:

$$\sum_{k=1}^{m+1} r_{ik}\pi_k + b_k u = \sum_{i=1}^{n} a_{ij} x_i^{(0)} f_i\left[X^{(0)}\right], \quad k = 1,\ 2,...,\ m+1 \qquad \text{(D.13)}$$

where:

$$r_{jk} = r_{kj} \equiv \sum_{i=1}^{n} \left(a_{ij} a_{ik}\right) x_i^{(0)} \qquad \text{(D.14)}$$

and

$$u \equiv \frac{\overline{x}^{(1)}}{\overline{x}^{(0)}} - 1 \qquad \text{(D.15)}$$

Eqs. (D.13) and (D.15) taken together represent a system of $m + 2$ linear equations in the unknowns $\pi_1, \pi_2, ..., \pi_{m+1}$ and u. After solving them, we can calculate the coefficients $x_1^{(1)}$, $x_2^{(1)}$,…, $x_n^{(1)}$ by means of Eq. (D.10). White *et al.*[5] also showed how to ensure non-negative values of the coefficients $X(p)$ = $\{x_1^{(p)}, x_2^{(p)},\ldots, x_n^{(p)}\}$ in each cycle, and proposed a very simple way for computing the concentrations of species present in traces.

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