Atmospheric Chemistry During the Accretion of Earth-like Exoplanets

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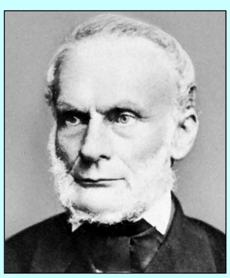
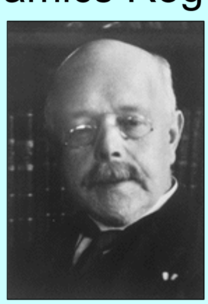
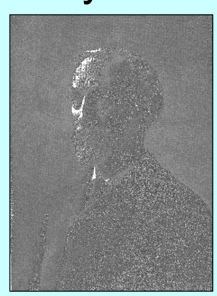
Thermodynamics Rogues Gallery



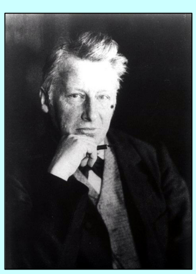
Rudolph Clausius



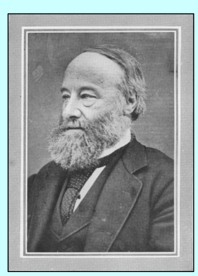
Walther Nernst



Willard Gibbs



Jacobus Van't Hoff



James Joule

Introduction

- Most terrestrial accretion theories suggest that the Earth was at least partially molten
  - Many accretion theories suggest that there was a magma ocean
- Giant impacts (e.g. Moon-forming impact) generate magma oceans which are hot enough to vaporize
  - There is new evidence for large impacts in exo-planetary systems (Song et al., Nature, July 2005)
- Therefore terrestrial-type planets should get hot (T > 2000 K) and vaporize during accretion
  - Vaporization generates silicate atmospheres containing gases such as SiO that may be detectable spectroscopically and condense into clouds

Accretional Energy

- Some theories suggest that a magma ocean formed as Earth accreted
  - Suggested magma ocean temperatures are > 2000 K
- Energy released by accretion of an Earth-like planet (1 $M_\oplus$ ~ 6 × 10^{24} kg & 1 $R_\oplus$ ~ 6370 km) is:

$$\frac{GM_\oplus^2}{R_\oplus} = \frac{(6.67\times10^{-11} m^3 kg^{-1} s^{-2})(6\times10^{24} kg)^2}{(6370\times10^3 m)} \sim 4\times10^{32} Joules$$

- Energy to heat up and vaporize bulk silicate Earth (BSE) is:

Liquidus temperatures for possible magma ocean

Magma type	T_{liq} (K)[1]	$T_{b.p.}$ (K)[2]
Tholeiite	1433	3270
Komatiite	1838	3341
Dunite	1954	3294
Forsterite	2163	3540
Bulk silicate Earth	1892	3361
Bulk silicate Mars	1844	3269

[1] computed using Magfox code
[2] computed using MAGMA code

$$E_{vap} = \frac{M_{BSE}}{\bar{\mu}} \times \Delta_{vap}H = \frac{(4\times10^{27} g)}{(140\ g\ mol^{-1})} \times 1180\ kJ\ mol^{-1} \sim 3\times10^{31} Joules$$

$$\frac{E_{accretion}}{E_{vap}} = \frac{GM_\oplus^2}{R_\oplus E_{vap}} = \frac{4\times10^{32} Joules}{3\times10^{31} Joules} \sim 10$$

⇒ **Accretion of an Earth-like planet easily vaporizes the silicate portion!**

Impact Energy

ΔE (J)	Size of impactor	Thermal effects
7×10^{27}	1.4×10^{20} kg (~mass of asteroid Pallas)	Boil oceans and heat to 2000 K
5×10^{28}	1×10^{21} kg (~mass of asteroid Ceres)	Melt crust and heat to 2000 K
2×10^{29}	4×10^{21} kg (~5% mass of Earth's moon)	Vaporize crust and heat to 3200 K
3×10^{31}	6.8×10^{23} kg (~mass of Mars)	Vaporize silicate Earth and heat to 3540 K

- **Giant impact models give temperatures of 4000 – 5000 K**
  - Some accretion models now suggest that impacts between large bodies may be ubiquitous
- **Kinetic energy ($\frac{1}{2}mv^2$) converts into thermal energy after an impact**
  - Thermal energy is used to sequentially heat up solids, melt solids, heat liquids, vaporize liquids, and then heat the gas
- **Assuming an impact velocity of 10 km s^{-1}, the energy of impact is:**
  - ΔE_{impact} (J) = $5\times10^7 M$, where M = mass of impactor (in kg)
  - Table illustrates the effects of various sized impactors
  - Cooling times for these impacts range from on the order of 10 years for the smallest impact to 10^3 – 10^4 years for the Mars-sized impact

Possible Extrasolar Terrestrial Planets

Planet	Mass
Earth	1 $M_\oplus$
Gliese 876d	7 $M_\oplus$
55Cnc e	14 $M_\oplus$
GJ436b	21 $M_\oplus$
HD160691d	14 $M_\oplus$
HD190360c	18 $M_\oplus$

- Several extrasolar terrestrial-size planets (see table).
  - **Indicates that terrestrial planet formation occurred in several other planetary systems**
- Also evidence for accretion of rocky material in the innermost 2 AU (terrestrial planet region) of three protoplanetary disks (van Boekel et al. 2005, Nature)

Methods

Model compositions for the magma ocean

Oxide (wt%)	BSE[1]	BSM[2]
SiO_2	45.56	45.39
MgO	36.33	29.71
Al_2O_3	4.73	2.89
TiO_2	0.178	0.14
FeO	8.17	17.22
CaO	3.75	2.35
Na_2O	0.349	0.98
K_2O	0.035	0.11

[1]BSE = Bulk Silicate Earth, from O'Neill & Palme (1998)
[2]BSM = Bulk Silicate Mars, from Lodders (2000)

- We used a thermochemical equilibrium model to calculate the composition of silicate atmospheres
  - Nominal magma ocean composition = dry bulk silicate Earth
  - Temperature range = 2000 – 5000 K
    - based on accretion, giant impact models, and energetic constraints
  - 40 gas and 42 melt species were included in our calculations
- check effect of volatiles (H & C) on the atmospheric chemistry
- use atmospheric adiabatic profiles for different atmospheric compositions
- derive the composition of condensate clouds in the silicate atmospheres

Dry Silicate Atmosphere (1)

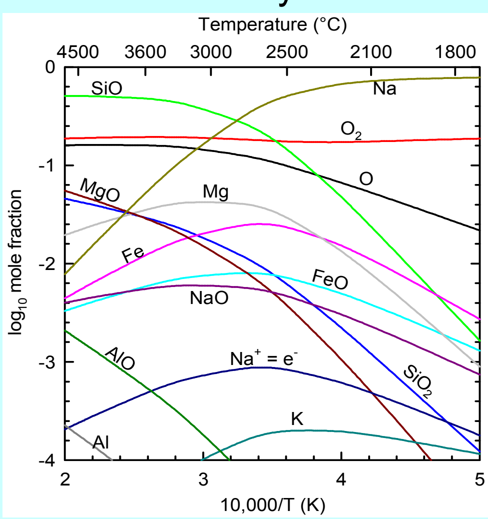


Fig. 1. Composition of a dry (no H, C) silicate atmosphere over a magma ocean with the composition of the bulk silicate Earth from 2000 – 5000 K

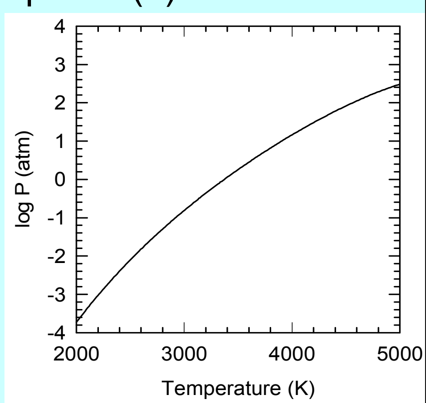


Fig. 2. Total vapor pressure of a dry silicate atmosphere over a magma ocean with the composition of the bulk silicate Earth from 2000 – 5000 K

Dry Silicate Atmosphere (2)

- Fig. 1 shows the silicate atmosphere composition for the dry bulk silicate Earth composition given in the table
- Major gases are Na for T < 3080 K and SiO for T > 3080 K
- The major Ca and Ti gases are Ca and TiO
  - These gases are not abundant enough to appear in the graph
- Major ions in the gas are:
  - Cations: Na^+ (~98.5 – 99.2%), K^+ (~1.5 – 0.8%) (% of total cations for T = 2000 K – 5000 K)
  - Anions: e^- (99.99% – 47 %), O^- (0.01% – 40%), O_2^- (<0.001% – 13%) (% of total anions for T = 2000 K – 5000 K)
- Total pressure of the atmosphere shown in Fig. 2:
  - $\text{Log } P_T \text{ (bar)} = 9.01 - 3.74\times10^4/T + 2.38\times10^7/T^2$
- Vaporization of a magma ocean causes chemical fractionation:
  - The atmosphere is enriched in volatile elements (e.g. Na, K) relative to the magma ocean

Wet Silicate Atmosphere

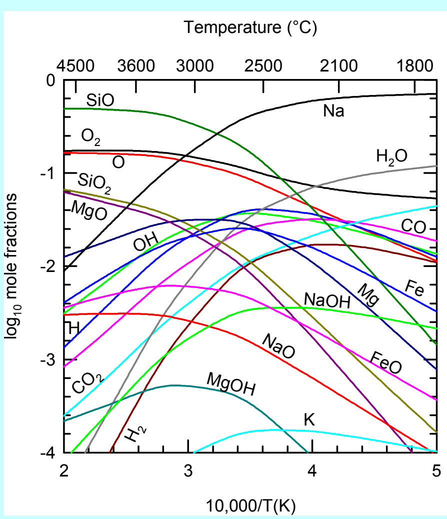


Fig. 3. Composition of a wet (H, C- bearing) silicate atmosphere over a magma ocean with the composition of the bulk silicate Earth from 2000 – 5000 K

- Composition of silicate atmosphere with H and C
  - atomic H/Na = 0.41 and atomic C/Na = 0.09 for the bulk silicate Earth
    - H_2O = 0.0413 wt% (oceans)
    - C = 0.012 wt%
- We assumed complete degassing of all H and C into the atmosphere
- We used same P and T as for dry atmosphere
- Major gas is SiO for T > 3080 K & Na for T < 3080 K
- H_2O is 2nd most abundant gas for T < 2500 K
- CO is more abundant than CO_2 for T > 2300 K

Adiabatic Atmospheric Profiles

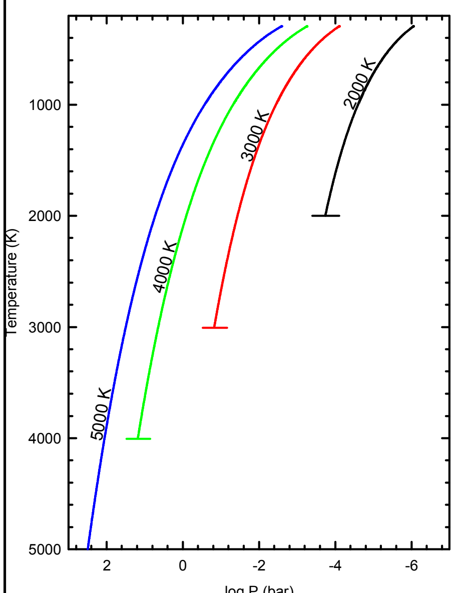


Fig. 4. Adiabatic profiles for silicate atmospheres with compositions taken from Fig. 1.

- Dry adiabatic P/T profiles for vapor over anhydrous magma ocean with the bulk silicate Earth composition
- Different profiles reflect different atmospheric composition based on magma ocean temperature

Magma ocean T	Atmosphere composition
2000 K	78% Na, 20% O_2, 2% O
3000 K	35% Na, 25% SiO, 18% O_2, 12% O, 4% Mg, 3% Fe, 3% other
4000 K	49%SiO, 19% O_2,16% O, 4% Na, 3% Mg, 3% MgO, 3% SiO_2, 1% Fe, 2% other
5000 K	50% SiO, 20% O_2, 17% O, 6% MgO, 5% SiO_2, 2% Mg

Cloud condensates (1)

Cloud compositions for 2000 K atmosphere

Cloud	T_{cond} (K)	Z (km)[1]
Mg_2SiO_4	1955	~4.5
$CaAl_2Si_2O_8$ (l)	1931	~7
$CaSiO_3$ (l)	1896	~9.5
SiO_2 (crist.)	1870	~13
Fe_3O_4	1817	~18
TiO_2	1602	~40
Na_2O	1169	~82

[1]calculated using the dry adiabatic lapse rate and terrestrial *g*

- Condensation sequence for the 2000 K atmosphere along the adiabat shown in Fig. 4.
- Size of clouds:
  1) **Most massive cloud is Na_2O; removes all Na from the gas**
  2) **SiO_2 (cristobalite)**
  3) **Fe_3O_4**
  4) **Mg_2SiO_4**
  – **$CaAl_2Si_2O_8$ (l), $CaSiO_3$ (l), TiO_2 produce only thin haze layers**
  – **K does not condense at any altitude**
- Table gives approximate altitudes (z) of the cloud base
- Holes in the clouds allowing observation of lower atmosphere would be indicative of weather

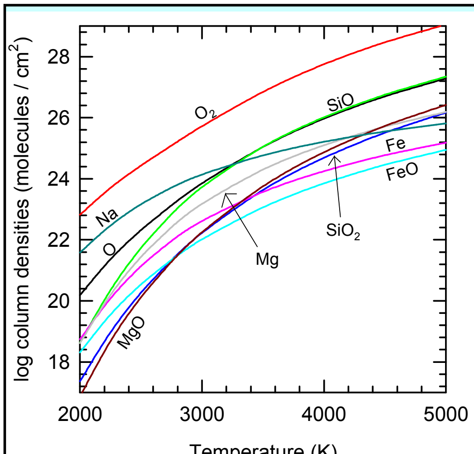
Cloud Condensates (2)

Cloud compositions for 5000 K atmosphere

Cloud	T_{cond} (K)	Z (km)[1]
$CaMgSi_2O_6$ (l)	4751	~26
$MgSiO_3$ (l)	4661	~35
Al_2O_3 (l)	4190	~84
SiO_2 (l)	4180	~85
FeO (l)	3618	~142
TiO_2 (l)	2852	~219
Na_2O (l)	1730	~330

[1]calculated using the dry adiabatic lapse rate and terrestrial *g*

- Condensation sequence for the 5000 K atmosphere along the adiabat shown in Fig. 4.
- Size of clouds:
  1) **Most massive cloud is molten SiO_2, which removes all Si from the gas**
  2) **MgSiO3 (liq)**
  3) **Na_2O (l)**
  – **$CaMgSi_2O_6$ (l), Al_2O_3 (l), FeO (l), and TiO_2 (l) produce only thin hazes**
  – **K does not condense at any altitude**
- Table gives approximate altitudes (z) of the cloud base
- **All condensates are liquids!**
  – Liquid droplets may have distinctive optical properties



Opacity of H-chondrite silicate vapor[1]

T(K)	P (bar)	λ	κ (cm^{-1})
3000	1	IR Visible	10^{-6} – 1 10^{-2} – 10
5000	100	IR Visible	0.1 – 100 2 – 3000

[1] Nemtchinov et al. 1997, *Icarus*, **130**, 259-274 (and references therein)

SiO gas has strong IR bands at 4 and 9 μm and lines throughout mm wavelengths

Possible SiO gas masers

– SiO masers are observed in circumstellar shells, molecular clouds, star-forming regions, and supernovae

– SiO has column densities from 10^{11} to 10^{15} cm^{-2} in these regions

- Silicate atmospheres above magma oceans have much higher column densities of SiO (shown in Fig.7. at left)

Photochemical lifetime of SiO for present day UV flux at 1 AU is ~4 min. at zero optical depth

– Based on stellar observations, UV flux in past was probably larger, giving an even shorter lifetime!

– However, silicate vapor is very opaque for high temperatures and pressures, so the actual lifetime of SiO should be much longer

Summary

- Energetic considerations show that enough energy is released during accretion to melt and vaporize an Earth-like terrestrial planet
- Terrestrial planets accreting around other stars should glow in visible to IR regions because their effective temperatures are similar to or greater than those of brown dwarfs such as Gliese 229b
  - During accretion, terrestrial planets have silicate atmospheres generated by vaporization of the accreting material
- Major species in the silicate atmospheres are Na, O_2, O, SiO, and if wet, also H_2O
  - SiO has strong bands at 4 and 9 microns and masers are possible in very hot silicate atmospheres
  - O_2 is abundant from silicate vaporization and may be observable
- Condensation clouds of liquid and/or solid oxides and silicates form in the silicate vapor atmospheres of hot Earth-like exoplanets