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to the  
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## General Introduction

This is the first annual technical report for research carried out under NASA Contract NASW-3477 by J. S. Lewis Associates, Inc., a not-for-profit corporation chartered in the Commonwealth of Massachusetts. The Corporation was founded for the purpose of carrying out basic research under contract to governmental and industrial clients, and is structured to carry out theoretical and computer modeling research using minicomputer technology rather than large mainframe computers. The Corporation will make every effort to keep overhead expenses as low as possible, and will encourage recent PhDs with excellent qualifications who are unable to find tenure-track university positions in the present depressed academic job market to seek research support under its aegis.

Our work during the first year of this contract has concerned three research areas of fundamental interest to the NASA planetary exploration program. These areas are the chemistry and physics of formation of the satellite system of Jupiter, the comparative study of the conditions of origin of Venus and Earth, and the condensation behavior of presolar solids in physically realistic astrophysical settings. Our progress in these areas is described in sections I, II and III of the present report, respectively. The accomplishments of the first year have closely approximated our original intent as expressed in last year's proposal; however, the means by which these ends were achieved have changed. It was our original proposal to rent a minicomputer at the outset of this work, choosing the most capable one for the available funds. However, at the time of the outset of this work it became known

that a new IBM system (the Personal Computer) would be on the market in a few months. Accordingly, we chose to begin this project by renting a terminal and buying time on a large computer. During the year the IBM computer came out, and we are now running on it in Basic, pending the availability and assessment of a FORTRAN compiler. We are delighted with the speed and capacity of this computer, and have nearly finished the task of program conversion.

Our cost experience during the first year reflects the nature of a newly begun program: secretarial expenditures have run low and late in the year because the burden of report preparation could only be begun once sufficient research had been done to write up. Since we have to date only submitted one report for publication, our publication expenses have so far been virtually nil. The budgeted travel money could not be used due to the untimely illness of the P. I. None of these circumstances should apply during the coming year, and the budget has been planned accordingly.

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## SECTION I

CHEMICAL AND PHYSICAL MODELS OF THE  
JOVIAN SUBNEBULA

John S. Lewis  
J. S. Lewis Associates, Inc.

**Abstract**

A semiempirical physical model of the Jovian subnebula has been developed by analogy with the primitive solar nebula itself. This model employs simple power-law scaling of the dependence of temperature, pressure, density and surface density with jovicentric distance. The chemical aspects of this model are developed according to the principles developed in the study of the thermochemistry and gas kinetic behavior of the solar nebula, but with important modifications to take into account the higher pressures and densities in the jovian subnebula. These differences in physical conditions are reflected both in the higher condensation temperatures of pure substances, and in the degree to which gas phase and heterogeneously catalysed gas reactions approach equilibrium. In the jovian subnebula, unlike the solar nebula, the reduction of the high-temperature gases CO and N<sub>2</sub> by reaction with molecular hydrogen can readily proceed toward equilibrium, thus making both NH<sub>3</sub> and CH<sub>4</sub> relatively more important components in the jovian system. The bulk compositions and densities of the inner satellites of Jupiter are calculated from this physico-chemical model and compared to observations. The recent petrological model of Io which attributes its active sulfur magmatism and sulfur dioxide venting to an initial state of rather high degree of oxidation is found to be reasonably concordant with this model. It is proposed that Europa differs from Io chiefly in that it has suffered a less severe thermal history. The general features of this model are applicable with minor modification to the systems of Saturn and Uranus.

## Introduction

Advancing theoretical understanding of the early history of the jovian system and in our observational data base for Jupiter and its satellites permits an attempt to use the geochemical modeling techniques which have been developed to treat the solar nebula in this narrower context. Perhaps the greatest shortcoming of any model for the early solar system is that it almost always contains certain ad hoc postulates or adjustable parameters which, however plausible and successful, may be utterly lacking in generality. Because of the nature of the observational evidence, we may not readily turn to another solar system to test our theory. Thus we are left quite uncertain whether we have a general scientific theory, or a mere engineering model of our own system which reflects many features we observe, but may lack essential physical insights into the fundamental processes at work.

The existence of regular satellite systems about Jupiter, Saturn and Uranus provides us with three new opportunities to expose our theories to test.

We shall here explore a very particular and simple analogy between the formation of the planets out of a primitive solar nebula and the formation of Jupiter's satellites out of a primitive jovian subnebula. While this model is in principle applicable to the systems of Saturn and Uranus as well, our

greatly superior knowledge about the jovian system compels us to test the model first in that context.

Following Cameron (1978) and others, we shall assume solar elemental abundances for the jovian subnebula. By analogy to the mass distribution in the solar nebula, computed by distributing the mass of each planet over a torus centered about the orbit of that planet, and replenishing missing volatiles up to solar relative abundances (Weidenschilling, 1977), we find a surface density,  $\sigma$ , which is proportional to the heliocentric distance,  $r$ , raised to the  $-1.6$  power. From the general dependence of planetary density and bulk composition on heliocentric distance, we find that the temperature in the solar nebula varied as  $r$  to the  $-1.1$  power (Lewis, 1974). These assumptions combine to require that the midplane nebular pressure,  $P_c$ , drops off as the  $-3.6$  power of the heliocentric distance, while the midplane gas density,  $\rho_c$ , drops as the  $-2.5$  power of  $r$ .

The densities of the Galilean satellites drop off monotonically with distance from Jupiter, in a fashion reminiscent of the behavior of the densities of the planets as a function of their distance from the sun. The masses and densities of the Galilean satellites are given in Table 1. By comparison with the theoretically computed bulk density of the condensed portion of a solar-composition system (Lewis, 1972, 1974), it is plainly evident that water ice must be a major component of both Ganymede and Callisto, but not Io and Europa. Accordingly, we shall place

Table I

Radii, Masses and Densities of the Galilean Satellites

Satellite	Radius (km)	Mass ( $10^{24}$ gm)	Density ( $\text{g/cm}^3$ )
Io	1820	89.1	3.53
Europa	1552	48.7	3.03
Ganymede	2635	149.0	1.93
Callisto	2420	106.5	1.83

the condensation threshold of ice halfway between the orbits of Europa and Ganymede. Now, using the nebular dependence of surface density and temperature on distance found above, and requiring that the surface density must be sufficiently high to provide the observed mass of the most massive Galilean satellite, Ganymede, we may then calculate the expected compositions, masses and densities of the other Galilean satellites and Amalthea (J5).

We assume for the sake of simplicity that condensed matter is accreted into that satellite whose orbit is closest to the point of origin of the solids: this assumption should be very good for the purpose of estimating the total accreted mass, but less adequate for describing the compositional diversity of each satellite (and hence its exact bulk density and volatile content).

Our procedure shall be to calculate first the temperature, pressure, and density profiles in the subnebula, and then to superimpose on this structure the condensation points of the rock-forming and ice-forming species in the nebula. We then calculate the bulk composition of each satellite, its mass, and its density. We then shall compare these satellite models to observational evidence. Finally, we shall critique the model both in light of the available evidence and the theoretical naivete of its assumptions.

### Physical and Chemical Structure of the Subnebula

Our results for the temperature profile in the jovian subnebula are given in Fig. 1. The temperatures at the present orbits of the inner jovian satellites are found to be about 1100K for Amalthea (at a pressure of about 80 bars), 450K for Io (4b), 275K for Europa (0.8b), 170K for Ganymede (0.16b), and 140K for Callisto (0.05b). The ice condensation point along this adiabat lies at 225K, ammonium hydrosulfide condenses at 170K, and ammonia monohydrate at 150K. The temperature given for Callisto is of course uncertain to some degree due to the uncertainty in determining exactly where the adiabatic thermal structure of the inner part of the subnebula gives way to the radiatively controlled and nearly isothermal outer portion of the subnebula. Thus it is far from certain that ammonia monohydrate would in fact condense and be accreted into Callisto.

While these results were being prepared for publication, a preprint on the same subject (Lunine and Stevenson, 1981) was sent out. Although the physical model of the nebula employed by Lunine and Stevenson was constructed to quite different criteria than the present model, the results are strikingly similar. In general, the temperature and pressure gradients in the present model are slightly steeper, while the temperatures and pressures of formation of each satellite are slightly lower.

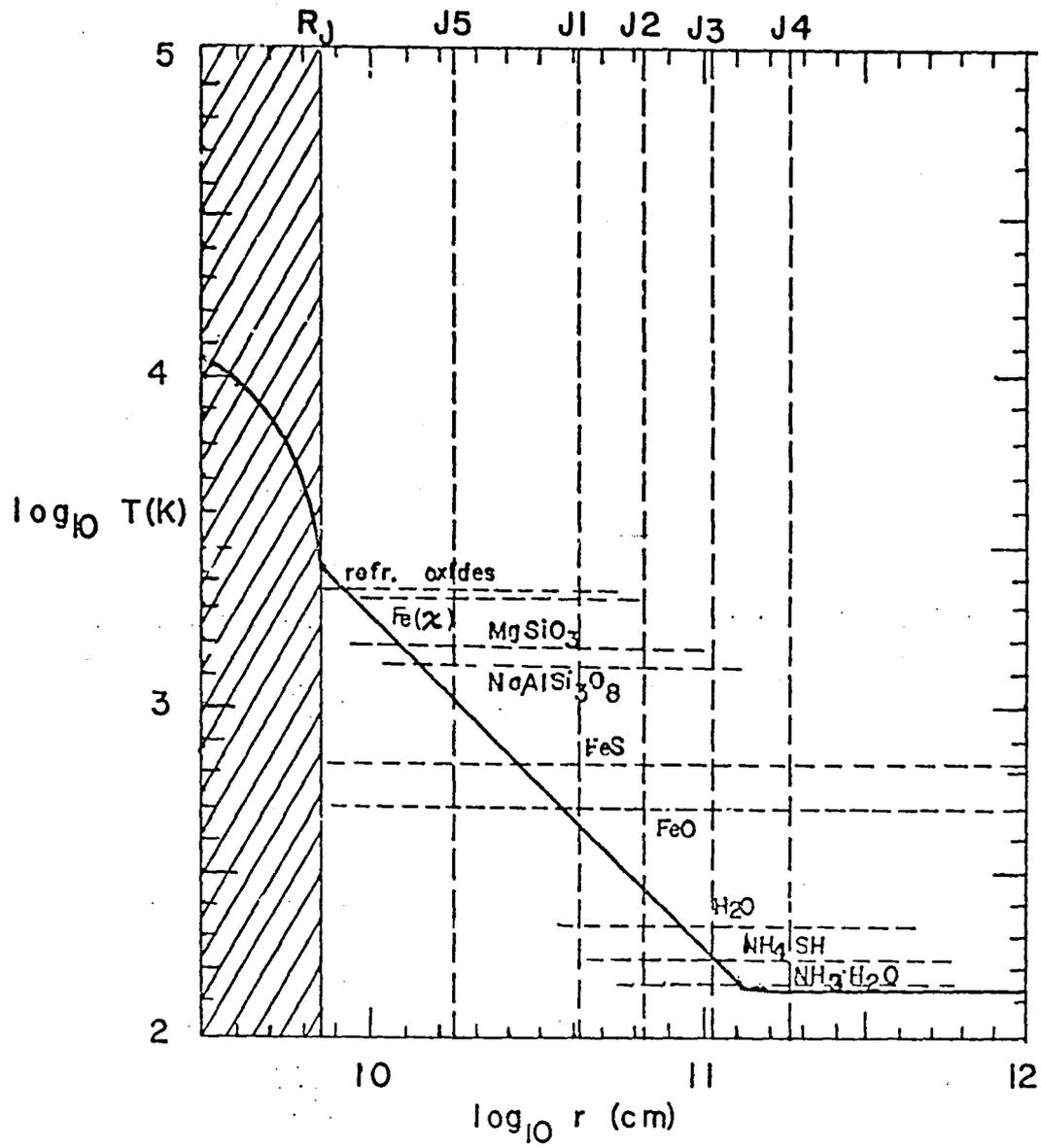
Since Lunine and Stevenson have concentrated on the composition relationships between Ganymede and Callisto, and since our

## Caption to Fig. 1

## Temperatures and Condensation Fronts in the Jovian Subnebula

The vertical solid line marks the present radius of Jupiter, and the vertical dashed lines mark the orbital semimajor axes of the five innermost large satellites, J5 (Amalthea), J1 (Io), J2 (Europa), J3 (Ganymede), and J4 (Callisto). The condensation points for refractory oxides, liquid metallic Fe-Ni, enstatite, albite, troilite, the endpoint for oxidation of Fe, and the condensation points of water ice, ammonium hydrosulfide, and the solid monohydrate of ammonia are indicated by the horizontal dashed lines. Condensation behavior is predicated upon the assumption of adiabatic structure and solar elemental abundances.

FIG. 1



results for these bodies, calculated for a nebular mass about half that used by them and for a slightly lower temperature, are strikingly similar, we shall concentrate on the predictions of this model for Amalthea, Io and Europa.

Our calculated condensation point for Amalthea lies well below the condensation curves of metal, magnesium silicates, and alkali aluminosilicates, but well above the formation temperature of troilite, FeS. A very highly reduced assemblage would be expected, in which kamacite and taenite would be abundant, but the FeO content of the principal silicate (enstatite) would be negligible. The relationships between the formation conditions of the inner satellites and the condensation curves of the rock-forming elements can be seen in Fig. 2. Note that the composition of Amalthea is predicted to be closely similar to that of Venus, even though the pressure at the point of formation of Amalthea is approximately 105 times higher.

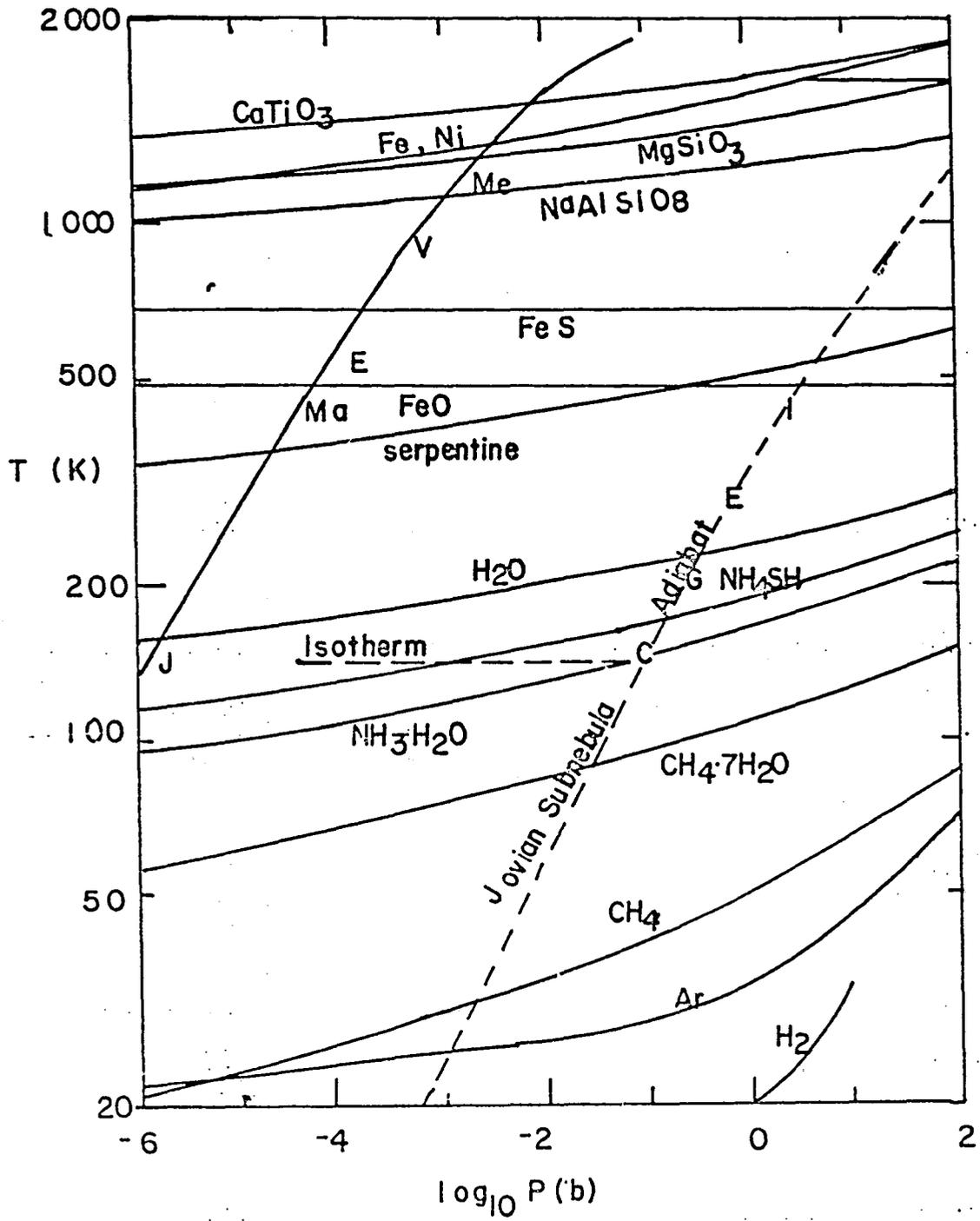
The composition of Io is expected to be closely similar to that of Mars, although with a higher initial water content due to the formation of the material of Io within the stability field of serpentine. Whether serpentine can be formed in the solar nebula by reactions between water vapor and ferromagnesian minerals is certainly debatable: it is more plausible to attribute the meteoritic occurrences of this mineral to secondary alteration reactions which took place on the meteorite parent body. The water vapor partial pressure in the jovian subnebula at the point

## Caption to Fig. 2

## Pressure-Temperature Structure of the Jovian and Solar Nebulae

The condensation curves of a number of species are given for a range of temperatures and pressures which spans those of interest in both the solar nebula (solid curve) and the jovian subnebula (dashed curve). The symbols on the solar nebula curve denote the conditions at the orbits of Mercury, Venus, Earth, Mars, and Jupiter at the time of maximum temperatures in the nebula. The symbols on the jovian subnebula adiabat denote similarly the condensation conditions at the orbits of Amalthea, Io, Europa, Ganymede, and Callisto. The jovian nebula is likely to be optically thin (and hence nearly isothermal) outside the orbit of Ganymede, as indicated by the horizontal dashed line. Condensation of ammonia hydrate in the jovian system is regarded as marginal at best, and may well not be possible.

Fig. 2



of serpentine formation is fully  $3 \times 10^5$  times as large as that in the nebula at the corresponding point in the condensation sequence. In addition, serpentinization in the subnebula becomes thermodynamically possible at about 600K, compared to 360K in the solar nebula. It is therefore entirely plausible that serpentine may form readily by gas-solid reactions in the subnebula, but that the kinetics of its formation in the solar nebula are prohibitively slow. The model strongly suggests that metallic iron will be rare or absent in Io, and hence that the oxygen fugacity will be buffered at far higher values than the Fe-FeO buffer.

A recent petrological model of Io (Lewis, 1981) discusses the conditions necessary for sulfur magma generation and sulfur dioxide-driven volcanism. In that discussion it is shown that the liquid sulfur magma and its driving gas must be derived from a source material devoid of metallic iron and rich in oxidized iron. It is further maintained that sulfur magmatism could not arise on Io until after loss of any primordial endowment of water and carbon dioxide. This massive loss of volatiles is energetically plausible for Io because of its strong tidal heating, but is extremely difficult for a cold, massive planet like Mars. It is for this reason that Mars and Io, even if they had identical initial compositions, would have followed divergent evolutionary paths.

The composition calculated for Europa lies slightly above the

water ice condensation curve, as required by our original constraints on the model. Thermal evolution of Europa as a closed system would cause decomposition of the phyllosilicate component, resulting in release of large quantities of water to the surface. This is a plausible source of the surface ice layer on Europa.

#### Critique of the Model

The first and most general test to which we may subject these results is to determine whether the absolute and relative masses of the Galilean satellites are acceptably in accord with observation. We can readily check the relative masses by augmenting the mass of each satellite up to full solar composition by replenishing the missing volatiles in solar proportions. The material of each satellite is then spread over an annulus centered about that satellite's orbit and extending halfway to the orbit of each of its two neighboring satellites. The surface density of this material projected upon the symmetry plane of the nebula can then be plotted and compared to the solar nebula model. Figure 3 presents the data on this mass distribution calculated as shown in Table 3. The slopes of several different power law relationships between the surface density and distance are shown for comparison. It can be seen that the actual mass distribution in the jovian system, when the actual densities and approximate compositions of the satellites are properly taken into account, fits a surface density which varies as the  $-2.3$  power of jovicentric distance, not the  $-1.6$  power as derived from analogy with the solar system. Note that Lunine and Stevenson calculate a theoretical slope

**Caption to Fig. 3****Radial Distribution of Mass in Jupiter's System**

The nebular density in the protojovian subnebula, calculated in the manner described in the text, is compared with four different functional relationships between the surface density and jovicentric distance. The mass distribution inferred in this manner is significantly steeper than that which was calculated theoretically by Lunine and Stevenson, or that found empirically for the solar nebula (see Table 4).

Fig. 3

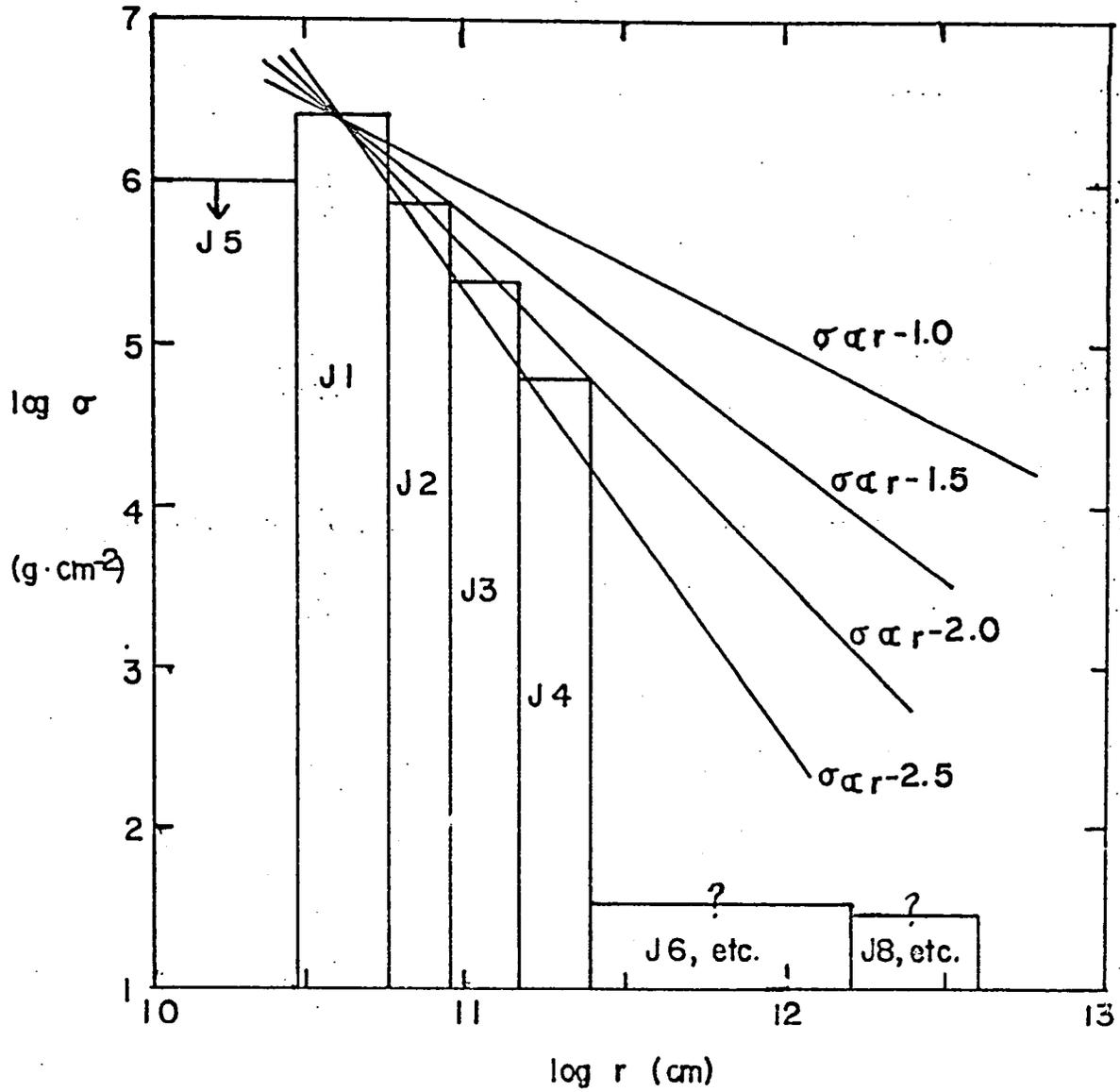


Table 3  
Minimum Mass of the Jovian Nebula\*

Satellite	Mass	Factor	M(solar)	r(annulus)	A(annulus)	Surface Density
Amalthea	<1	~240	<240	1.81	27	<1,000,000
Io	89.1	210	18700	4.22	67	2,790,000
Europa	48.7	200	9740	6.71	143	680,000
Ganymede	149.0	80	11900	10.71	440	270,000
Callisto	106.5	80	8520	18.83	1285	66,000
J6,7,10 each	<1	80	<200	116.	70000	<30

\* Masses in  $10^{\frac{24}{3}}$  g, radii in  $10^{\frac{10}{-2}}$  cm, area in  $10^{\frac{20}{2}}$  cm<sup>2</sup>, surface density in  $10^{\frac{3}{-2}}$  g.cm<sup>-2</sup>.

of about  $-1.5$  from their model of the dynamics of the nebula. We may attribute the discrepancy either ignorance of the fluid mass distribution in the jovian nebula or, more plausibly, to the very severe modification of the original distribution of solids by the effects of frictional drag between small particles and the very dense gas. A naive assessment of the effects of drag would surely attribute the most severe drag effects to condensates in the densest (innermost) portions of the nebula, and hence it would be reasonable to expect that friction would broaden and flatten the initial distribution of solids. This is the opposite to the effect actually observed. An alternative possibility is that the rate of accretion is so phenomenally high in the inner portion of the subnebula that bodies rapidly accrete to sizes large enough to be insensitive to drag effects.

In order to make clear the basis for these comparisons between the solar nebula and the jovian subnebula, it is necessary to include a specific and explicit model for the distribution of matter in the solar nebula. Such a model, based on recent ideas regarding the compositions of the jovian planets, is given in Table 4. The mass factors needed to convert an observed solid body of approximately known composition into its solar-composition counterpart are shown in Table 5.

Table 4

## Minimum Mass of the Solar Nebula\*

Planet	Mass	Factor	M(solar)	r(annulus)	A(annulus)	Surface Density
Mercury	3.3	448	1480	0.33-0.83	1.82	813.
Venus	48.7	238	11590	0.83-1.29	3.06	3788.
Earth	59.8	223	13325	1.29-1.89	6.00	2220.
Mars	6.4	216	1382	1.89-3.20	20.95	66.
(ast.)	(<0.1)	200	(<20)	3.2-6.0	80.9	<0.3
Jupiter	14040.	5	70200	6.0-11.0	267.	262.
Saturn	5695.	12	68380	11.0-21.5	1072.	64.
Uranus	870.	44	38230	21.5-36.8	2802.	13.7
Neptune	1032.	50	51600	36.8-52.0	4240.	4.6
Pluto	0.01	80	<1	52-70	6900.	

\* Masses in  $10^{26}$  g, radii in  $10^{13}$  cm, area in  $10^{26}$  cm<sup>2</sup>, surface density in g.cm<sup>-2</sup>.

Table 5

Mass Factors for Condensates in a Solar-Composition System

Category	No. of Moles (Si=1)	Mass	Mass Fraction $x(i)$ of Solar Mix	Factor (=1/x)
Dry rock		196.0	0.0047248	212.
FeO	0.600	43.2	0.0010414	
FeS	0.400	35.2	0.0008485	
MgO	1.060	42.4	0.0010221	
SiO <sub>2</sub>	1.000	60.0	0.0014464	
CaO	0.072	4.2	0.0001012	
Al <sub>2</sub> O <sub>3</sub>	0.042	4.3	0.0001037	
Ni	0.048	2.6	0.0000627	
Na <sub>2</sub> O	0.030	1.9	0.0000458	
All others	-	2.2	0.0000530	
Ices		577.0	0.013909	72.
H <sub>2</sub> O	17.80	320.4	0.007724	
NH <sub>3</sub>	3.74	63.6	0.001533	
CH <sub>4</sub>	11.80	188.6	0.004546	
Ar	0.12	4.4	0.000106	
Gases		40710.	0.981365	1.019
H <sub>2</sub>	15900.0	31800.	0.766580	
He	2210.0	8840.	0.213099	
Ne	3.4	70.	0.001687	
Total		41483.	1.000000	1.000

It is not presently possible to subject the compositional predictions of this model to very demanding tests, due to the fact that our present knowledge of the compositions of the Galilean satellites is limited to bulk densities and some (literally) superficial spectroscopic data. Several of the few available compositional constraints have already been mentioned in the previous pages, and no conflict between these limited data and the predictions of the present model is evident.

#### Directions for Future Research

The behavior of the solids present in the dense jovian subnebula is of great interest. I have indicated above the existence of evidence for important radial transport of solids in the subnebula, presumably as a result of frictional dissipation caused by the velocity difference between solids and the embedding gas. This inward evolution of the solids, combined with the very short synodic periods of bodies in nearby orbits and the very high densities of dust and gas in the inner regions of the subnebula, suggest strongly that a detailed study of the dynamics of orbital evolution and accretion of solids in this system would be of great value. Interestingly, recent advances in the treatment of the motion and accretion of solids in the solar nebula both in the United States and Japan have provided a basis for such modeling. Further, the interesting question of the vapor and condensed phase transport mechanisms in the solar nebula has become the subject of a joint effort by myself and R. G. Prinn (funded through grants to

M.I.T.), and will surely be of great importance in the jovian subnebula. In this study, the outward eddy transport of vapors across condensation fronts, partly balanced by the inward evolution of solid bodies due to viscous drag, leads to complex and markedly nonuniform distributions of condensables in the system. Application of this approach to the jovian subnebula, once the principle has been worked out for the solar nebula, would not be difficult.

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SECTION II

VENUS: HALIDE CLOUD CONDENSATION  
AND VOLATILE ELEMENT INVENTORIES

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and  
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**Abstract**

Several recently suggested Venus cloud condensates, including  $Al_2Cl_6$  as well as halides, oxides and sulfides of arsenic and antimony, are assessed for their thermodynamic and geochemical plausibility. Aluminum chloride can confidently be ruled out, and condensation of arsenic sulfides on the surface will cause arsenic compounds to be too rare to produce the observed clouds. Antimony may conceivably be sufficiently volatile, but the expected molecular form is gaseous  $Sb_2S_3$ , not the chloride. Arsenic and antimony compounds in the atmosphere will be regulated at very low levels by sulfide precipitation, irrespective of the planetary inventory of As and Sb. Thus the arguments for a volatile-deficient origin for Venus based on the depletion of water and mercury (relative to Earth) cannot be tested by a search for atmospheric arsenic or antimony.

Soviet spacecraft have analysed cloud particles in the main Venus cloud layer by means of x-ray fluorescence (XRF) spectroscopy (1). These analyses claim detection of Cl as a cloud constituent, with S not detected. These in situ results are in conflict with the weight of evidence from Earth-based studies (2) and from other spacecraft experiments (3), which strongly suggest that the dominant cloud constituent on Venus is  $H_2SO_4$  droplets. Satisfactory photochemical models for the production of an  $H_2SO_4$  aerosol from geochemically plausible primary gases, including COS,  $H_2S$  and  $SO_2$  are available (4). Unfortunately, direct evidence regarding the abundances of these species in the lower troposphere is lacking: copious production of COS, etc. by reactions between sulfuric acid and the inlet system of the mass spectrometer on the Pioneer Venus large probe leads to masking of the atmospheric sulfur gases, and abundances up to 100 ppm are possible for COS and  $H_2S$  (5).

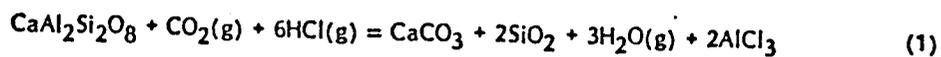
The source of a chlorine-bearing aerosol is less obvious. We have previously pointed out the high volatility of halides and sulfides of mercury, arsenic and antimony (6), and have shown that the terrestrial crustal abundance of even the rarest of these elements, Hg, would suffice to produce substantial masses of halide cloud condensates on Venus: mercury is so volatile at the surface temperature of Venus that it would reside almost completely in the atmosphere.

More recently, in the context of a model for the formation of the planets in the presence of a steep gradient outward from the proto-Sun, we have favored compositional models in which the volatile elements are severely depleted in the accreting Venus relative to Earth (7). The failure of the 1978 Pioneer Venus mission to detect even a trace of Hg in the lower atmosphere (5) strongly implies that Venus is deficient in Hg relative to Earth. The severe depletion of the most abundant terrestrial volatile,  $H_2O$ , on Venus is well known, and is variously attributed to either a lack of water in pre-planetary solids at the orbit of Venus (7,8) or to massive loss of oceans worth of  $H_2$  after differentiation and outgassing of the planet (9). Such a late loss mechanism could not, of course, deplete mercury while leaving vast amounts of the lighter and more volatile species  $N_2$  and  $CO_2$ . Thus the observed severe depletion of Hg on Venus is more convincing evidence for a volatile-poor high-temperature origin of Venus than is the depletion of water. Other moderately volatile elements, such as arsenic, antimony, bismuth and germanium are also potential indicators of the overall volatile content of Venus. In addition, such species, if present in the hot lower atmosphere would condense at intermediate altitudes to form solid halides, sulfides, and oxide cloud particles.

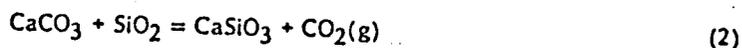
In the past year, Krasnopolsky and Parshev (10) have suggested  $Al_2Cl_6$  as the major cloud layer constituent, and Barsukov et al (11) have suggested arsenic and antimony halides and oxides. Mole fractions of 0.1 to 1 ppm of condensible gases are required to provide the

observed cloud density (12). Are these species plausible cloud constituents? Can useful limits on the abundances of the volatile elements As and Sb be derived from atmospheric measurements?

It is a simple matter to estimate the volatility of aluminum compounds at the mean surface conditions of Venus. Consider co-existing anorthite ( $\text{CaAl}_2\text{Si}_2\text{O}_8$ ), quartz ( $\text{SiO}_2$ ) and calcite ( $\text{CaCO}_3$ ) at 750 K and 95 bars in contact with the atmosphere:



The equilibrium constant for this reaction at this temperature is  $10^{-26.1}$ . Assuming the spectroscopic HCl abundance in the clouds, about 1 ppm (13), and the most typical water vapor abundance figures for the lower atmosphere, about 100 ppm (14), an  $\text{AlCl}_3$  partial pressure of  $10^{-21.0}$  b is calculated. With an extreme effort to bias the equilibrium in favor of  $\text{AlCl}_3$  production (raising HCl to 10 ppm and lowering  $\text{H}_2\text{O}$  to 10 ppm), we can force the  $\text{AlCl}_3$  pressure only as high as  $10^{-16.5}$  b. This is still 10 orders of magnitude too small to provide detectable amounts of condensate. Note that the presence of granitic rocks on Venus, with anorthite and quartz as common primary minerals, is expected both from consideration of the atmospheric composition (15) and from surface passive gamma-ray spectroscopy (16). The surface of Venus lies, as accurately as can be determined, precisely on the calcite-quartz-wollastonite ( $\text{CaSiO}_3$ ) buffer:



and calcite is therefore also a plausible surface mineral. Since weathering reactions at higher altitudes on Venus will preferentially tend to mobilize a fine Ca-rich dust, which can be transported readily by winds to the hot lowlands, this buffer may in fact not be difficult to establish on Venus (17).

Thermodynamic treatment of arsenic and antimony volatilization can be carried out without a precise a priori knowledge of the minerals formed by these elements on the surface (18,19). We shall calculate the partial pressures of a number of As and Sb gases at the surface as a function of the activities of As and Sb: an activity of one means the pure element is present on the surface; and activity of  $10^{-4}$  means that the pressure of the monatomic vapor of that element is  $10^{-4}$  times its abundance at saturation. We can then assess the stability of possible surface minerals containing these elements. Fig. 1 presents the results for arsenic (20). For As activities greater than about  $10^{-2}$  the dominant gas is  $\text{As}_4$  with  $\text{As}_4\text{O}_6$  second. Based on the

**Captions of Figures**

Fig. 1. Partial pressures of arsenic gases as a function of elemental arsenic activity at the Venus surface. Limitations of the arsenic activity imposed by precipitation of liquids of  $As_2S_3$  (orpiment) and  $As_4S_4$  (realgar) composition are indicated by the vertical dashed lines. Heavy dots indicate the upper limits on the  $As_4$ ,  $As_4O_6$ , and  $AsS$  partial pressures. A condensible species with a partial pressure near  $10^{-4}$  bars is needed to provide the observed cloud density. The maximum total mole fraction of arsenic gases is  $\leq 0.1$  ppm.

Fig. 2. Partial pressure of antimony gases as a function of elemental antimony activity. The  $Sb_4O_6$  (valentinite) and  $Sb_2S_3$  (stibnite) precipitation points are indicated by the vertical dashed lines. Firm upper limits on the antimony gas pressures are indicated by the dots. The maximum total mole fraction of antimony gases is about 0.03 ppm. An  $SbS$  gas abundance of 0.3 ppm is needed to make clouds.

Fig. 1

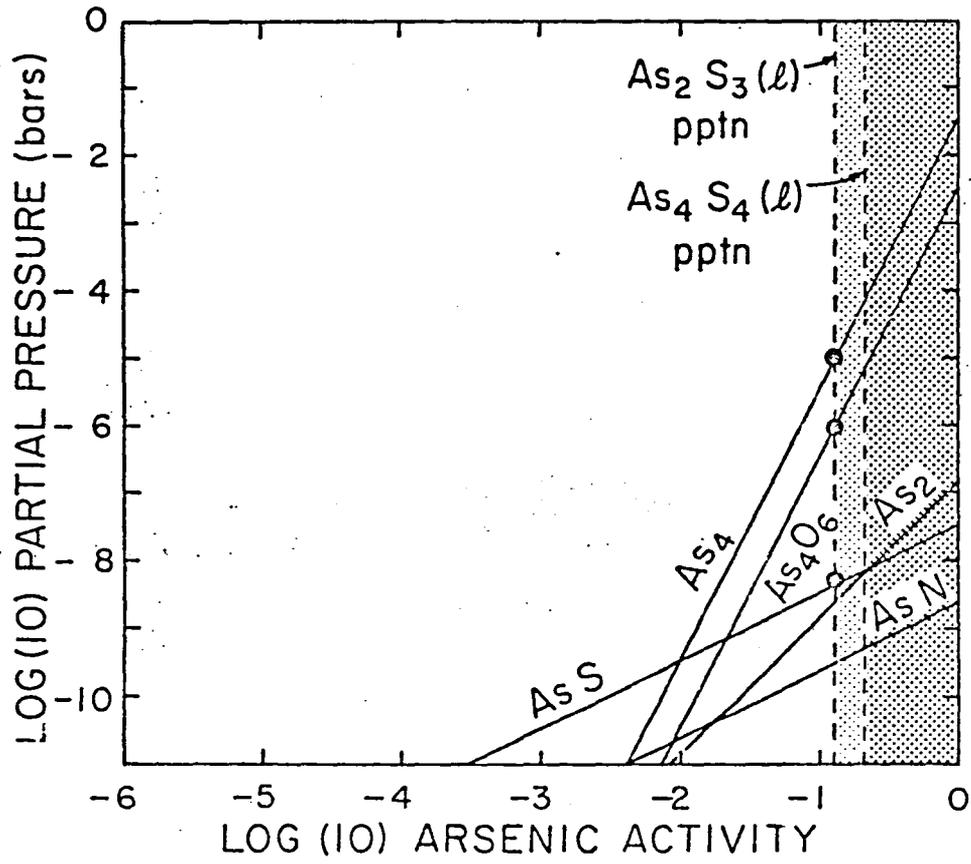
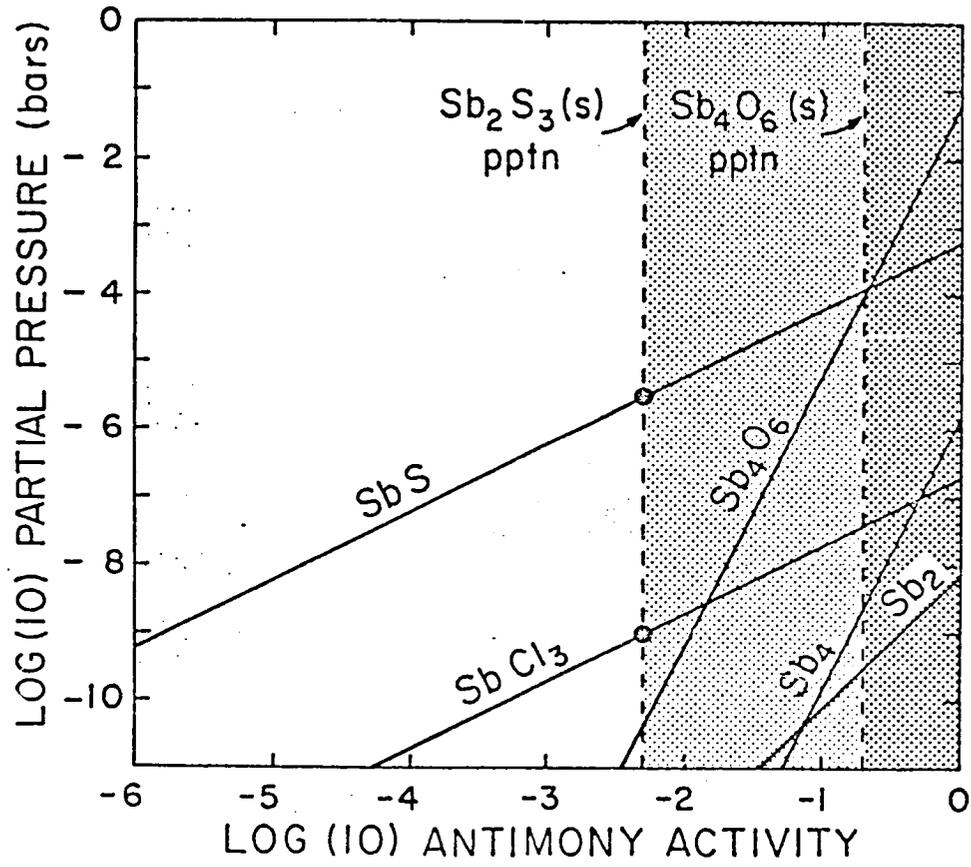


Fig. 2



recent thermochemical data of Johnson et al (18), we calculate that liquid  $As_2S_3$  will precipitate if the elemental arsenic activity is greater than 0.13, thus ruling out higher As activities. This in turn places firm upper limits on the pressures of As-bearing gases as indicated in Fig. 1.

The results of a similar calculation for antimony are given in Fig. 2. Precipitation of  $Sb_4O_6(s)$  occurs for an elemental antimony activity of 0.20. Thus for all possible Sb activities,  $SbS$  is the dominant gas. The best available data on  $Sb_2S_3$  (stibnite) from Johnson's work (18) indicate that  $Sb_2S_3(s)$  precipitates at an antimony activity of  $10^{-2.3}$ . Therefore we expect that stibnite precipitation on the Venus surface will regulate the Sb gas phase abundance.

We conclude that the mole fraction of all arsenic gases is below  $10^{-7}$ , probably making these species too rare to account for the clouds no matter what species condenses. We expect that the total mole fraction of antimony gases will be lower than for arsenic, but that the most stable gas is  $SbS$ , not a halide. Partial pressures as high as  $10^{-4}$  bars are conceivable for  $SbS$  and cannot be confidently ruled out.

Observational constraints on the abundance of arsenic in the Venus atmosphere even down to the level of 0.1 parts per million are therefore not sufficient to test whether arsenic is, like water and mercury, depleted in Venus relative to Earth: the stability of arsenic sulfides is great enough to preclude a larger abundance of gaseous arsenic compounds irrespective of the crustal abundance of As. The same may be true of antimony, since the mineral  $Sb_2S_3$  seems to have low enough volatility to hide Sb in the lithosphere. We have also briefly considered bismuth, and find that  $Bi_2S_3$  is so stable that the most abundant Bi bearing gas,  $BiS$ , should have a mole fraction below  $10^{-12}$ .

In any event, we call into serious question the geochemical plausibility of all the species so far suggested as sources of chlorine-bearing clouds. We suggest that either the chlorine compound is a species which has not been considered, or the XRF data used to deduce the presence of chlorine may be in error (21).

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19. The P, T, composition conditions assumed in these calculations are 95 bars total pressure, 750 K surface temperature,  $P_{O_2} = 10^{-22.5}$  bars,  $P_{HCl} = 10^{-4.0}$  bars,  $P_{S_2} = 10^{-4.0}$  bars, and  $P_{HF} = 10^{-5.2}$  bars.
20. Other As- and Sb-bearing gases included in the calculations but which are not abundant enough to be graphed are As, AsO, AsH<sub>3</sub>, AsF, AsF<sub>2</sub>, AsF<sub>3</sub>, AsF<sub>5</sub>, AsCl, AsCl<sub>2</sub>, AsCl<sub>3</sub>, Sb, SbO, SbH<sub>3</sub>, SbN, SbF<sub>3</sub>. The solid and liquid arsenic oxides As<sub>2</sub>O<sub>4</sub>, As<sub>2</sub>O<sub>5</sub>, and As<sub>4</sub>O<sub>6</sub> are unstable and do not precipitate as pure condensates on the surface of Venus. Formation of more complex minerals, e.g. As-bearing apatites and complex Sb oxides, for which thermodynamic data are unavailable, may result in lower gas phase abundances for As and Sb. Thus our results are firm upper limits.
21. We thank the Planetary Atmospheres and Planetary Geophysics and Geochemistry (NGR-22-007-269 to A.G.W. Cameron) program offices of NASA for support of this work through grants to J.S. Lewis Associates, Inc. and to A.G.W. Cameron, Harvard College Observatory. We thank Dr. G.K. Johnson for providing his Sb<sub>2</sub>S<sub>3</sub> data prior to publication. B.F. also thanks A.G.W. Cameron for support and facilities.

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SECTION III

ISOLATED GRAIN CONDENSATION BEHAVIOR:  
COMPUTATION METHODS AND FIRST RESULTS

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**Abstract**

A set of efficient programs for calculation of condensation behavior in a system with either solar or carbon-rich elemental composition has been developed to treat the course of condensation at very low pressures. Condensation processes of astrophysical interest, such as those occurring in the atmospheres of C stars and in nova and supernova envelopes, can be treated by these programs. These programs have been applied to the problem of condensation at very low pressures, where intergrain collisions are rare and nucleation sites for silicates are found only on the surfaces of previously condensed grains. This "isolated grain" case gives results which diverge in interesting ways from both the equilibrium condensation and the nonhomogeneous accretion models.

Extension of the programs to a set of 20 elements is under way, and a full set of publishable results for the condensation process in the above cases of astrophysical importance will soon be available. This project is also producing calculation procedures which make it possible to carry out complex thermochemical equilibrium calculations using a small computer.

The minerals produced in the stellar and nova-related processes under study, including carriers of important volatile elements such as carbon and nitrogen, are candidates for accretion into meteorite parent bodies and planets, and may still be discernible in the enstatite chondrites.

## Introduction

Considerable work has been done during the past year on the condensation behavior of a solar-composition gas in cool stellar environments and in carbon-rich astrophysical environments such as C nova shells. These environments are the original sites of condensation of the solids in interstellar clouds and preplanetary nebulae, and hence are the ultimate sources of the solids present in the solar nebula. The first phase of this project concentrated on developing FORTRAN programs to treat the gas and condensation chemistry of solar material, with the novel constraint that reactions between two or more dissimilar grains and the cooling gas were omitted. This corresponds to the physical condition that grains formed in astrophysical settings generally do so at extremely low pressures, usually less than 0.01 dynes per square centimeter. Thus nucleation sites are at a premium, grains almost never collide, and condensation takes place at unusually low temperatures. Therefore fresh condensates tend to coat old grains, and diffusion is very slow. Disequilibrium between the solids in the grain interiors and the gas is enhanced by the high diffusion barrier, but also by the short dynamic expansion and cooling times inherent in nova and supernova ejecta and in carbon star "smoke". Some of the early condensates, especially in systems with an excess of carbon over oxygen, are excellent candidates as carriers of volatile elements, especially carbon and nitrogen.

The puzzling departures from equilibrium seen in certain classes of meteorites, especially the carbonaceous chondrites and

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the enstatite chondrites, point strongly to non-nebular processes. In the case of the carbonaceous chondrites, secondary alteration processes in a parent body have become widely accepted. Secondary alteration processes have also been proposed to explain the strange coexistence of very highly reduced high-temperature silicates with abundant volatiles and low-temperature sulfides in the enstatite chondrites, but this scenario has not been generally accepted. Both classes, in fact, contain carbon and other highly reduced phases which suggest origins in astrophysical settings different from the classical simple-minded picture of a solar composition nebula. As mentioned in Section I, we have already begun to look at gas and dust transport processes in a dynamical model of the solar nebula to see whether such transport may contribute to the stability of the odd phases in chondrites. The present project deals with the possibility that these odd grains may have been inherited from a presolar interstellar cloud without extensive chemical alteration.

#### Program Development and Computation Strategy

During the initial phase of this project, calculations were carried out from a terminal leased by the company, using the Multics system at the MIT computer center. An arrangement was made by which c. p. u. time would not be charged on this project. That arrangement was withdrawn by MIT last summer, so that after-hours work was necessary to realize reasonable rates. With the availability of the new IBM Personal Computer, it became possible to remove all computation from large, expensive systems

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and thereby do away with connect-time and cpu-time charges. This was so attractive a possibility that we immediately translated some of the fundamental computation routines into Basic for use on the IBM. This conversion was carried out very efficiently, and we are now running in Basic. A FORTRAN compiler has been announced for the IBM, but is not yet commercially available.

The present strategy employs gas equilibration routines which can be stepped in both temperature and pressure, and which calculate the condensation thresholds of a number of solid phases. The program is run interactively, so that the appearance of a new condensate can be screened for its stability under the rules of the procedure (isolated-grain behavior), and accordingly accepted or rejected.

The computer programs used in this project differ substantially from the free-energy-minimization routines which have become widely used. They have the advantage that they are readily adaptable to use on small computers without using excessive core, and that under almost any circumstances they compile and execute in a fraction of the time. The procedure is an iterative improvement of elemental activities (initially estimated by a kind of programmer chemical intuition) in which the magnitude of the corrections to the activities is determined by the comparison of the total computed abundances of the compounds of each element to the initially specified elemental abundance of that element. A pressure-temperature point can be solved in a system of 16 elements within one to two minutes by the IBM Personal Computer, and this performance can be realized with programs which have not

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been purged of several obviously inefficient (but reliable ) procedures. The Basic program is now being expanded to 20 elements, which is the size of the largest FORTRAN program of this general type so far developed (the program TOP20, developed by S. S. Barshay while he was a student of mine at MIT, which could only be run on CDC6600 or larger computers!). The problem of exponent overflow and underflow, a perennial issue with IBM computers, can be completely and efficiently bypassed by a new scaling procedure which we have developed this year.

We have already reported briefly on some of the features of the isolated-grain condensation process in our renewal proposal, and we include here a summary of the more interesting features of this process which set it apart from the more familiar equilibrium condensation process.

#### Results to Date

The general features of the isolated-grain condensation process which we have documented to date include important differences in the behavior of iron and the alkali metals. The nature of the condensation sequence can best be appreciated by comparing the results to the more conventional equilibrium condensation and nonhomogeneous accretion schemes.

The first condensates in all three schemes are refractory oxide minerals rich in aluminum, calcium, and titanium and poor in silicon. These include corundum, spinel, perovskite, anorthite and melilite solid solution. The next condensate in all three schemes is metallic iron-nickel alloy. The third condensate is

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magnesium silicate. At high total pressures, forsterite is the first magnesium silicate to appear, followed by alteration to enstatite by reaction with silicon-bearing vapors at slightly lower temperatures. At pressures of 0.1 dyne per square cm, the condensation temperature of iron has dropped below that of enstatite, so that enstatite slightly precedes metal as a condensate. The equilibrium condensation model predicts that all of the silicon will be used up in forming silicates, with none left over to form quartz. However, both the nonhomogeneous accretion model and the isolated-grain model effectively paint lower temperature condensates on high temperature condensates. Thus the former process rapidly accretes forsterite, then enstatite, then quartz onto growing planetesimals, while the latter similarly zones individual grains. The alkali feldspars require intimate contact between gas, anorthite, and a silica-rich phase such as quartz. This is prevented in the nonhomogeneous accretion scenario by early accretion and burial of anorthite, and in the isolated-grain model by the coating of anorthite grains (the main source of aluminum) by impervious layers of magnesium silicates and silica.

Note that, up to this point, the likely mineral products of the nonhomogeneous accretion and isolated grain models are essentially identical. The difference lies in the way that these mineral components would be distributed in a planetesimal: the nonhomogeneously accreted body will of course be strongly layered, with a core rich in refractories and metal, and a silica-rich surface. A body accreted from the products of isolated-grain

condensation would be chemically homogeneous on a distance scale of millimeters. An important point is that the equilibrium condensation products are quite distinct from those in either of these two schemes, and more closely resemble ordinary chondrites, in that they contain two feldspars, no free silica, and have significant traces of FeO in the olivine and pyroxene.

At this point the nonhomogeneous accretion and isolated grain condensation sequences diverge very significantly. Metallic iron is of course buried and chemically isolated from the gas in the former model, but present as metallic grains in the latter. Thus, at the appearance temperature of troilite (680K), it is possible for the isolated-grain process to make FeS unless silicates have nucleated on the metal grains. In view of the presence of silicate grains at all temperatures at which metal is condensed, it is plausible that nucleation of lower-temperature silicates will strongly favor these silicates, and thus not coat metal grains.

Phosphorous, like sulfur, should react in the isolated grain case with metal grains, but, due to the limited ability of these grains to absorb phosphorous and retain it at lower temperatures, phosphates should be ultimate products in all three schemes IF calcium were chemically available to form phosphates.

The issue of the behavior of phosphorous, along with the complex sequence of possible phases involving the alkali sulfides and halides, is still under study.

The following program listing is illustrative of the present level of development of the Basic translations and adaptations of our original FORTRAN programs, which were suitable only for use on very large computers.

```

10 READ BH, BHE, BO, BC, BN, BSU, BNE, BAR
11 READ BSI, PFE, BMG, BAL, BCA
20 FOR NT = 1 TO 10
25 READ T, KH, KH20, KCO, KCH4, KCO2
26 READ T, KOH, KO, KC, KH2S, KHS, KN
27 READ T, KCN, KHCN, KNH3, KS02, KS
28 READ T, KSI0, KSI, KSIH4, KFE, KMG
29 READ T, KCA, KAL, KALO
40 READ T, KSI02, KMGSIO3, KMG0, KMG2SIO4
41 READ T, KFES, KFESIO3, KFE2SIO4, KFEO
42 READ T, KAL203, KCA0, KSPINEL, KAN.25
50 FOR NP = 1 TO 10
59 F = 10!^(NP-10!)
60 ABH = F*BH
61 ABHE = F*BHE
62 ABO = F*BO
63 ABC = F*BC
64 ABN = F*BN
65 ABSU = F*BSU
66 ABNE = F*BNE
67 ABSI = F*BSI
68 ABFE = F*BFE
69 ABMG = F*BMG
70 ABAL = F*BAL
71 ABCA = F*BCA
72 ABAR = F*BAR
80 REM INITIAL GUESS OF ELEMENTAL ACTIVITIES
81 RH = -(KH/4)+SQR(KH^2+8*ABH)
82 RN = -(KN/4)+SQR(KN^2+8*ABN)
83 RO = (2*ABO)/(3*KH20*RH^2)
84 PH2 = RH^2
85 GR = ABC/((KCO*RO)+(KCH4*PH2^2))
86 RS = ABSU/((KS02*RO^2)+(KH2S*PH2))
90 ASI = ABSI/(KSI0*RO)
92 AMG = ABMG/KMG
93 AAL = ABAL/KAL
94 ACA = ABCA/KCA
99 INDEX = 0
200 FOR ITER = 1 TO 150
201 INDEX = INDEX+1
202 PH = KH*RH
203 PH2 = RH^2
204 FHE = ABHE

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211 PCH4 = KCH4\*GR\*PH2^2  
 212 PCO2 = KCO2\*GR\*RO^2  
 213 PC = KC\*GR  
 220 POH = KOH\*RH\*RO  
 221 PH2O = KH2O\*PH2\*RO  
 222 PO = KO\*RO  
 223 PO2 = RO^2  
 230 PCN = KCN\*GR\*RN  
 231 PHCN = KHCN\*GR\*RH\*RN  
 232 PNH3 = KNH3\*RN\*PH2\*RH  
 233 PN2 = RN^2  
 234 PN = KN\*RN  
 240 PH2S = KH2S\*RS\*PH2  
 241 PSO2 = KSO2\*RS\*PO2  
 242 PHS = KHS\*RH\*RS  
 243 PS = KS\*RS  
 244 PS2 = RS^2  
 250 PSIO = KSI0\*ASI\*RO  
 251 PSI = KSI\*ASI  
 252 PSIH4 = KSIH4\*ASI\*PH2^2  
 258 AFE = ABFE/KFE  
 259 IF AFE>1! THEN 260 ELSE 264  
 260 PFE = KFE  
 261 PMETFE = ABFE - PFE  
 262 AFE = 1!  
 263 GOTO 270  
 264 PFE = ABFE  
 265 PMETFE = 0!  
 270 PMG = ABMG  
 280 PCA = ACA\*KCA  
 281 PAL = AAL\*KAL  
 282 PALO = KALO\*AAL\*RO  
 300 REM CALCULATE ACTIVITIES OF SOLIDS  
 301 ASIO2 = KSI02\*ASI\*PO2  
 302 AMGSI03 = KMGSI03\*AMG\*ASI\*PO2\*RO  
 303 AMGO = KMGO\*AMG\*RO  
 304 AMG2SI04 = KMG2SI04\*AMG^2\*ASI\*PO2^2  
 305 AFESI03 = KFESI03\*AFE\*ASI\*PO2\*RO  
 306 AFE2SI04 = KFE2SI04\*AFE^2\*ASI\*PO2^2  
 307 AFES = AFE\*KFES\*RS  
 308 AFEO = KFEO\*AFE\*RO  
 320 ACAO = KCAO\*ACA\*RO  
 321 AAL2O3 = KAL2O3\*AAL^2\*PO2\*RO  
 322 ROOTAN = KAN.25\*PO2\*SQR(AAL\*ASI\*SQR(ACA))  
 323 AAN = ROOTAN^4  
 324 ASPINEL = KSPINEL\*AMG\*AAL^2\*PO2^2  
 400 REM CALCULATE ELEMENTAL SUMS  
 401 SH = PH+2\*PH2+2\*PH2O+4\*PCH4+3\*PNH3+POH+PHS+PHCN+2\*PH2S  
 402 SC = PCO+PCO2+PCH4+PC+PHCN+PCN  
 403 SO = PH2O+2\*PO2+2\*PCO2+PCO+POH+2\*PSO2+PSIO+PO+PALO  
 404 SN = FN+2\*FN2+PNH3+FCN+PHCN  
 405 SS = PS+PHS+PSO2+PH2S+2\*PS2  
 410 SSI = PSIO+PSI+PSIH4  
 411 SMG = PMG  
 412 SFE = PFE + PMETFE  
 413 SAL = PAL+PALO  
 414 SCA = PCA  
 419 P = PH2+PH+PH2O+PCO+PCO2+PCH4+PN2+PNH3+POH+PSIO+PFE+PMG+PH2S+PHE+PO+PNE+PHS+  
 PAL+PCA+PALO+PAR  
 420 EH = ABS(SH-ABH)/ABH  
 421 EO = ABS(SO-ABO)/ABO  
 422 EC = ABS(SC-ABC)/ABC  
 423 EN = ABS(SN-ABN)/ABN  
 424 ES = ABS(SS-ABSII)/ABSII

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431 EFE = ABS(SFE-ABFE)/ABFE
432 EMG = ABS(SMG-ABMG)/ABMG
433 EAL = ABS(SAL-ABAL)/ABAL
434 ECA = ABS(SCA-ABCA)/ABCA
440 IF EH<.001 THEN IF EO<.001 THEN IF EC<.001 THEN IF EN<.001 THEN IF ES<.001 T
HEN IF ESI<.001 THEN IF EFE<.001 THEN IF EMG<.001 THEN IF EAL<.001 THEN IF ECA<
.001 THEN GOTO 501 ELSE GOTO 449
449 REM COMPARE ELEMENTAL SUMS TO ABUNDANCES
450 IF INDEX = 1 THEN 451 ELSE 455
451 AFE = AFE*(ABFE/SFE)
452 RH = RH*SQR(ABH/SH)
453 AAL = AAL*(ABAL/SAL)
454 GOTO 500
455 IF INDEX = 2 THEN 456 ELSE 460
456 RN = RN*SQR(ABN/SN)
457 RO = RO*(ABO/SO)
459 GOTO 500
460 IF INDEX = 3 THEN 461 ELSE 465
461 AMG = AMG*(ABMG/SMG)
462 GR = GR*(ABC/SC)
463 ACA = ACA*(ABCA/SCA)
464 GOTO 500
465 RS = RS*(ABSU/SS)
466 ASI = ASI*(ABSI/SSI)
496 INDEX = 0!
500 NEXT ITER
501 REM OUTPUT RESULTS OF ITERATION
502 BEEP
505 PRINT "TEMPERATURE = ";T, "PRESSURE = ";P, ITER;"ITERATIONS"
507 PRINT "          PRESSURES OF GASES IN BARS"
508 PRINT "H =";PH;" H2 =";PH2;" HE =";PHE;" NE =";PNE;" AR =";PAR
509 PRINT "O =";PO;" O2 =";PO2;" OH =";POH;" H2O =";PH2O
510 PRINT "N =";PN;" N2 =";PN2;" NH3 =";PNH3;" CN =";PCN
511 PRINT "C =";PC;" CO =";PCO;" CO2 =";PCO2;" CH4 =";PCH4;" HCN =";PHCN;" SO2 =";
;PSO2;" ALO =";PALO
512 PRINT "S =";PS;" S2 =";PS2;" HS =";PHS;" H2S =";PH2S
513 PRINT "FE =";PFE;" MG =";PMG;" CA =";PCA;" AL =";PAL
514 PRINT "SIO =";PSIO;" SI =";PSI;" SIH4 =";PSIH4
516 PRINT "          ACTIVITIES OF CONDENSATES"
517 PRINT "OZ =";ASIO2;" MGO =";AMGO;" EN =";AMGSI03;" FO =";AMG2SI04;" FE =";
;AFE;" CAO =";ACAO;" COR =";AAL2O3
518 PRINT "FEO =";AFEO;" FS =";AFESI03;" FA =";AFE2SI04;" FES =";AFES;" SP =";ASP
INEL;" AN =";AAN
520 PRINT "          INPUT ABUNDANCES OF ELEMENTS"
521 PRINT "H =";ABH;" O =";ABO;" C =";ABC;" N =";ABN;" S =";ABSU
522 PRINT "FE =";ABFE;" SI =";ABSI;" MG =";ABMG;" AL =";ABAL;" CA =";ABCA
523 PRINT "          CALCULATED ABUNDANCES OF ELEMENTS"
524 PRINT "H =";SH;" O =";SO;" C =";SC;" N =";SN;" S =";SS;"CA =";SCA
525 PRINT "FE =";SFE;" SI =";SSI;" MG =";SMG;" AL =";SAL
545 INPUT GOON
546 IF GOON = 1 THEN 590 ELSE 650
590 NEXT NP
600 NEXT NT
650 END

```

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OF POOR QUALITY.

#### Directions for Future Work

Our efforts during the first year of this contract have been concentrated on writing and translating the computer programs to carry out the task, and only recently have we reached the point where publishable scientific calculations may be carried out. It is our expectation that the crucial scientific questions involving the details of the isolated-grain condensation process and the comparison of this process with previously explored scenarios can all be addressed directly within a month or two.

We therefore plan to examine the condensation processes for minerals in both solar-composition and carbon-rich systems at very low pressures, in accordance with our original proposal. It will then be a simple matter to compare these results to the observed mineralogy of meteorites to see whether such materials have persisted to the present. We are especially interested in identifying mineral carriers for the volatile elements, especially sulfur, carbon, nitrogen and the halogens because of their possible importance in contributing atmophile elements to the accreting terrestrial planets, including the possibility that some of the carriers of rare gases in meteorites may have originally condensed in astrophysical, rather than solar nebular, settings.

END

DATE

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JUN 17 1982

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