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FINAL TECHNICAL REPORT

to the

NATIONAL AERONAUTICS AND SPACE ADMINISTRATION

Planetary Atmospheres Program

on

CONTRACT NASW-3625

for the year

15 May 1982 to 15 May 1983

from

J. S. Lewis Associates, Inc.

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CONTENTS

General Introduction

This is the final report on a program of research designed for execution on microcomputers. At its original inception, the program was intended to run for a period of three years, and to involve

a. theoretical work on compositional trends in the systems of the Jovian planets, including both the radial chemical variations within each satellite system and the compositional trends from Jupiter through Saturn and Uranus to Neptune,

b. geochemistry of the moderately volatile elements on Venus, for the purpose of determining whether the Pioneer Venus and Venera compositional measurements within the Venus troposphere can reveal whether Venus originally had a volatile element inventory comparable to that of Earth, or whether it has always been deficient in volatiles, and

c. examination of several types of chemical processes of astrophysical interest, including condensation in cool stellar atmospheres and low-density nova shells, in which grains condense and cool in isolation, and grain-grain reaction products may be negligible, and also including the disequilibrium chemistry of such ejected interstellar matter under the influence of supernova shock waves in star-forming regions.

The original program of research was shortened by NASA to two years. In that time we have pursued all three of these projects to a considerable degree, but of course have left a number or loose ends that will be picked up under the continuation of this research at the University of Arizona. Our achievements are as follows:

a. We developed detailed physico-chemical models of the Jovian subnebula (as described in last years report) which were completed at the same time that Lunine and Stevenson of Cal Tech submitted a very large paper on the same subject. Although the chemical aspects of the problem were more closely studied in our work, and the physical aspects treated more thoroughly in Lunine and Stevenson's paper, the overall results are quite closely comparable. The largest differences in the results arise from relatively minor details of the mass and mass distribution in the Jovian subnebula, and are not important. We then turned our attention to the planetary side of the problem, examining the evidence for departures from solar composition in the envelopes of Jupiter and Saturn. Such departures may be due to fractionation processes during the era of planetary accretion, or to some form of differentiation within the planets once they have formed. For Jupiter, the evidence favors minor enrichment of carbon (and possibly nitrogen) over solar composition, and possible severe depletion of oxygen below its solar abundance by a factor of 10 to 100. We have examined the molecular composition of a suite of Jovian model atmospheres of non-solar composition, including studying the chemical effects of lightning discharges on the atmospheric chemistry, using the Voyager lightning results as the standard on which the calculations were based. The major results of this study are included in Section I of the present report. They will be submitted for publication in Icarus in the near future. We find that modest enhancements of C and N may serve to explain the observed presence of HCN in the Jovian troposphere, and that the production of organic matter by disequilibrium processes (shock wave heating) is only modestly larger than in a solar-composition atmosphere.

b. Our study of the geochemistry of Venus has culminated in a paper published in Science during the past year. A copy of that paper is included as Section II of the present report. Further planned work on the evolution of the hydrogen isotopic evolution of the Venus atmosphere, taking into account the known meteoritic and cometary mass fluxes through the inner solar system, has been deferred for future investigation at the University of Arizona. With the arrival of Shailendra Kumar at the U. of A. next year, and with the interest and involvement of Don Hunten, this project should continue to move forward.

c. We reported our initial work on the subject of condensation of preplanetary matter in low-density astrophysical settings in last year's report. Since then we have concentrated our efforts on the carbon chemistry of shocked interstellar cloud material, in an attempt to see whether conditions in star-forming regions are dependent upon photochemistry for the production of complex organic matter, or whether shock-wave heating from supernova explosions might be important in dense (optically opaque) clouds. The results, although still not complete, are very promising. Some of the features of this exploratory work are described in

Section III of the present report. Both aspects of this study (isolated-grain condensation and shock chemistry of the interstellar medium) will culminate in publications within the next few months.

After two of the originally planned three years, two of our three main projects have resulted in papers, one of which has already appeared in Science. We believe that work of this sort, done in this manner, is potentially a very cost-effective way for NASA or other agencies to get basic research done. It was our original purpose to start up this project for the purpose of providing a base of operations for young recent Ph. D.'s who are unable to find academic appointments under the present condition of the academic job market, and who would be lost to space science permanently if they had to seek employment elsewhere. We still believe that this principle is valid, but the premature termination of this productive project renders such a goal impossible.

I

Non-Solar Compositional Models of the Troposphere of Jupiter

Since 1969 it has been usual to assume that the elemental compositions of the tropospheres of Jupiter and Saturn are very close to that of the Sun. However, in recent years a number of interpretations of Earth-based and spacecraft-based infrared spectra of these planets have appeared which suggest significant departures from solar composition.

The most impressive such departure that has been suggested is for water vapor. Interpretations of IR spectra in the 5um transmission window suggest that there is insufficient water to saturate the atmosphere at temperatures above about 220K (Hanel, et al., 1979). When the 5um flux was qualitatively regarded as due to emission from small regions devoid of clouds,and therefore presumably dominated by very dry descending air, this observation presented no obvious conflict with the assumption of overall solar compositon for the troposphere. However, recent work indicates that the 5um emission may originate from a deep level within the troposphere over most or all of the planetary surface, and that this flux is attenuated by a thick, variable overlying atmosphere that must be dry everywhere on the planet down to levels where the temperature is 250 K or higher. The most careful available interpretations of the 5um spectrum (Bjoraker, et al., 1981; Drossart and Encrenaz, 1982) suggest that water vapor must be depleted by a factor of 100 or more below the solar abundance ratio of H2O:H2 = 1.3x10-3 throughout the troposphere. This would have an important effect on both the atmospheric molecular composition and the cloud mass and structure. It also would greatly change the amount and composition of organic compounds produced by disequilibrating processes such as lightning.

A second suggested departure from solar composition has been reviewed by Wallace and Hunten (198x), who summarize and criticize evidence from spectroscopic studies by Cochran (1977), Sato and Hansen (1979), and others. Recent work by Encrenaz and Combes (1982) and other post-Voyager results summarized therein suggest a 2- to 4-fold enrichment of methane in Jupiter and up to a 6-fold enrichment of methane in Saturn (Buriez and de Bergh, 1981).

A third, more subtle issue, is whether ammonia might be slightly enriched on Jupiter. It is likely that an enhancement of more than about a factor of two would make itself known through its effect on the microwave opacity of the troposphere, resulting in lower brightness temperatures in the centimeter region (Gulkis and Poynter, 1976). We shall consider ammonia abundances of 1 to 2 times the solar abundance.

Finally, phosphine appears to be enriched above solar proportions in Saturn by a factor of 1.5 or 2 (Tokunaga, et al., 1980; Larson, et al., 1980), but to have about 0.5 to 1 times its solar abundance in the upper troposphere of Jupiter (Drossart and Encrenaz, 1982). The latter authors conclude that the spectroscopic determinations of phosphine in the 5um and 10um regions are consistent with a solar phosphine abundance in the lower troposphere, modified by destruction of phosphine near the tropopause by solar UV photolysis (Prinn and Lewis, 1975).

We must recall that the observed amounts of phosphine on both Jupiter and Saturn near their tropopauses are not expected on the basis of strict equilibrium calculations on a solar-composition atmosphere, since a solar water vapor abundance would cause complete oxidation of phosphine to condensable phosphates at all temperatures below about 600K (Barshay and Lewis, 1978; Lewis and Fegley, 1981). However, it is kinetically plausible that, in a rapidly convecting atmosphere, oxidation of phosphine would quench near 800K, leaving most of the phosphine unoxidized (Prinn and Lewis, 1975).

The only other chemically active element so far identified spectroscopically, germanium (as the hydride germane), appears to have slightly less than its solar abundance on Jupiter, in accord with theoretical expectations (Lewis and Fegley, 1981).

The present paper reports on the molecular composition of Jovian model atmospheres in which carbon is enriched by a factor of five, and nitrogen by a factor of two, relative to the Sun. The consequences of several different oxygen depletion factors, from 10 to 10^5 times below solar abundance, are explored.

We shall examine the equilibrium composition of such a non-solar-composition atmosphere along a plausible Jovian adiabat, the likely effects of quenching of equilibration in rising parcels of gas, and the effects of lightning discharges on the abundances of trace constituents of such an atmosphere. Our method of calculation is basically that used by Lewis (1969), Barshay and Lewis (1975), and Lewis and Fegley (1981), adapted to run in BASIC on a microcomputer system. The method of treatment of the chemical effects of lightning is that used by Lewis (1980), scaled to the level of lightning activity deduced by Borucki, et al. (1982).

Equilibrium Composition

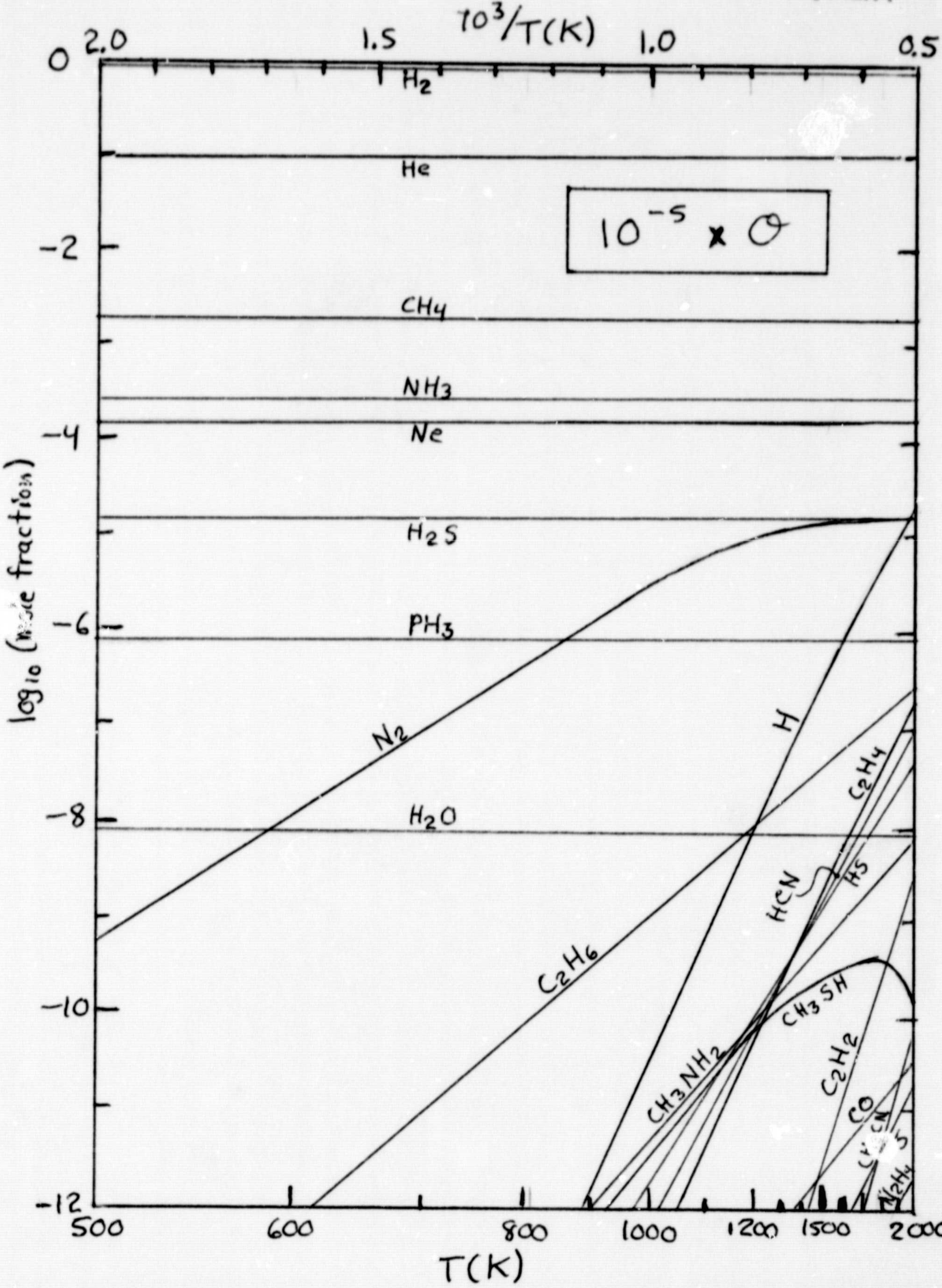
The mole fractions of a number of species at equilibrium along a Jovian adiabat are displayed in Figs. 1 and 2 for two different degrees of depletion of oxygen. All important oxygen compounds (water vapor, CO, formaldehyde, etc.) are depleted by the same factor that total oxygen is depleted: there are thus no important changes in the distribution of oxygen between its compounds, only in the overall abundance of this subset of compounds. Nitrogen compounds are raised in abundance by a factor of two for each N atom per molecule: thus ammonia is enhanced in abundance by a factor of two, and the relatively rare molecular nitrogen by a factor of four. Carbon compounds are enhanced by a factor of five for each C atom per molecule. Thus CH3CH2CH2CN would be enhanced by a factor of 625x2 = 1250 relative to its abundance in a solar-composition gas. Since some models of the atmospheres of Uranus and Neptune assume C:H ratios up to 1000 times the solar ratio, the extension of such calculations to these planets can be expected to yield much higher equilibrium concentrations of complex species than any chemical models of Jupiter and Saturn have included to date.

The model atmosphere in Fig. 1 (with a 10^5-fold depletion of oxygen) could not generate a distinct water cloud layer, and the ammonia clouds would be about twice as dense as in standard solar-composition models. Saturation of both solid ammonia and solid ammonium hydrosulfide would occur at a slightly higher temperature than in the solar-composition case. Aside from the

Caption to Fig. 1

Molecular abundances along a Jovian adiabat at chemical equilibrium, with oxygen depleted by a factor of 10^5, carbon enriched by a factor of 5, and nitrogen enriched by a factor of 2. The results for many other compounds under these conditions and at a variety of other conditions are given in the Appendices.

Fig. 1


$10^3/T(K)$
2.0
1.5
1.0
0.5
0
-2
-4
-6
-8
-10
-12
500
600
800
1000
1200
1500
2000
T(K)
$\log_{10}$ (mole fraction)
$10^{-5} \times O$
H_2
He
CH_4
NH_3
Ne
H_2S
PH_3
N_2
H_2O
C_2H_6
H
C_2H_4
HCN
HS
CH_3SH
CH_3NH_2
C_2H_2
CO

trivial enrichments of methane and ammonia and depletion of water, the only departures from the composition of an equilibrium solar-composition atmosphere visible at temperatures below 300K would be an increased N_2 abundance. However, the molecular nitrogen abundance in the upper troposphere is surely not regulated by local equilibrium, but rather by quenching of nitrogen reduction in rising parcels of gas (Barshay and Lewis, 1978).

The atmosphere in Fig. 2, with only a 10-fold depletion of water, would indeed form a water ice cloud layer with significant optical thickness. However, it may also provide more than the observed amount of water vapor near the ~250K level. Aside from these effects due solely and directly to the water vapor abundance, the observable properties of these two model atmospheres would be very similar. They would, however, differ significantly under the effects of lightning discharges: oxygen-bearing products such as carbon monoxide and formaldeyde would be produced in significant amounts in the latter case, but not in the former.

Note that the presence of phosphine at $T<600K$ is fully compatible with complete chemical equilibration if insufficient water vapor is available to oxidize all the phosphine. This will be the case if the water vapor abundance is less than 1.5 times the phosphine abundance. This occurs if water is depleted by a factor of 10^3 or more. Thus any atmospheric composition which provides a guarantee of phosphine stability would be incapable of generating detectable traces of CO due to rapid overturn. In this case, an exogenic source for CO must be sought (see, for example,

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Caption to Fig. 2

Molecular abundances along a Jovian adiabat at chemical equilibrium, with oxygen depleted by a factor of 10, carbon enriched by a factor of 5, and nitrogen enriched by a factor of 2. The dashed branches of the curves for phosphine and phosphorus sesquioxide assume exact equilibration, and are not likely to be attained during the convective overturn time. See the text for discussion.

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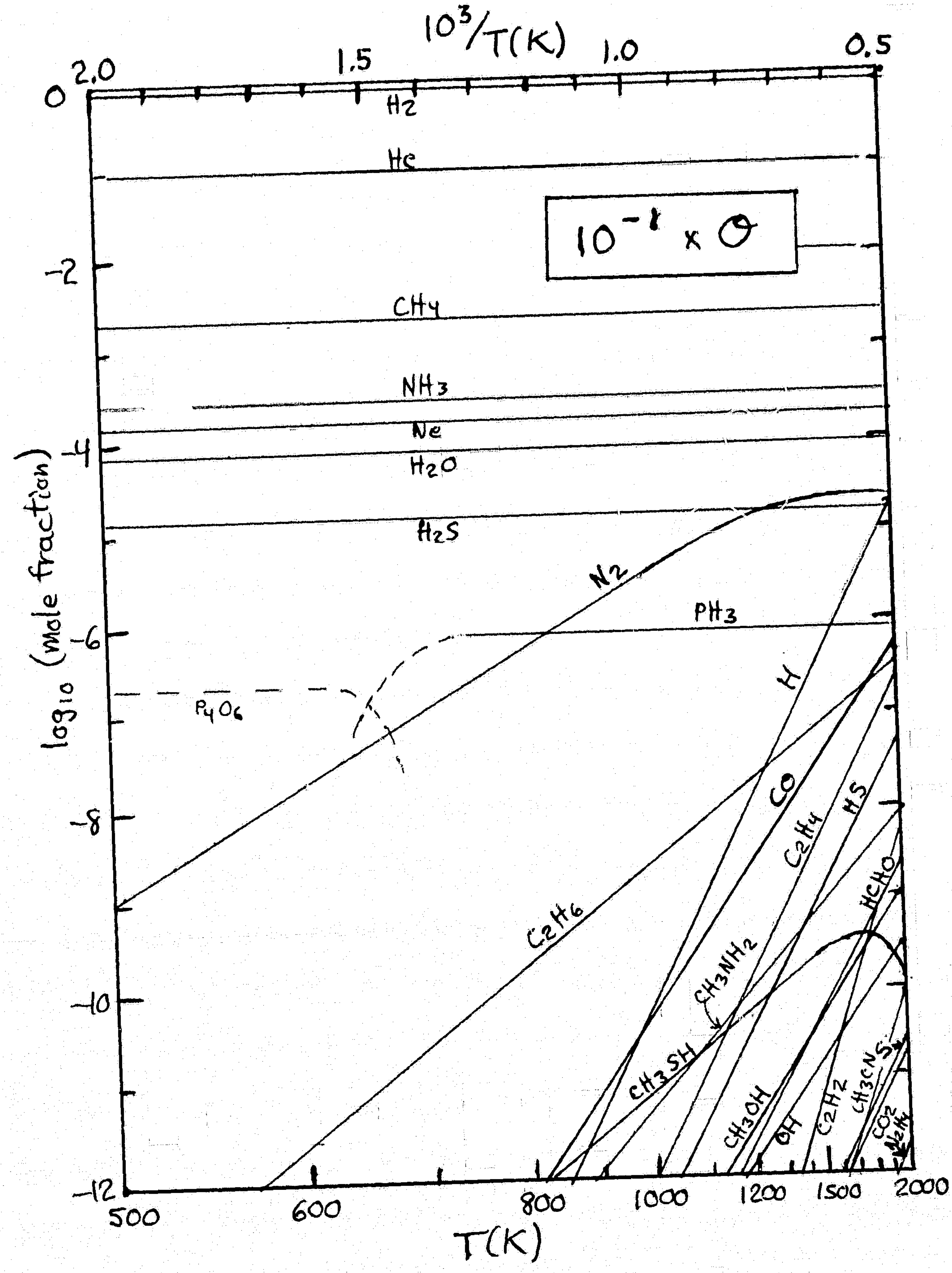
Fig. 2



Prather and McElroy, 1980; Strobel and Yung, 1980).

The observed presence of a trace of germane could easily be removed by reaction with hydrogen sulfide to precipitate GeS in any of these models, irrespective of the degree of water depletion. In all these models, as in the solar composition case (Barshay and Lewis, 1978; Lewis and Fegley, 1981), the observed presence of GeH_4 near the tropopause must be attributed to departures from equilibrium at low temperatures.

Quenching During Vertical Mixing

Kinetic arguments have been presented which suggest that quench temperatures near 1000K are reasonable for the reactions destroying many high-temperature species, such as CO, GeH_4, PH_3, HCN, acetylene, etc. (Prinn and Lewis, 1975; Prinn and Barshay, 1979; Lewis and Fegley, 1981; and the review by Lewis, 1983). For nitrogen, quench temperatures of 1000 to 1500K would result in a mole fraction of 4 to 12 ppm N_2. Quench of C_2H_6 destruction at 1000 to 1200K would provide 1.5 to 10 ppb of ethane at higher altitudes.

The only three oberved species that can plausibly be attributed to quenching of hot lower tropospheric gases due to rapid vertical mixing in an adiabatic solar-composition atmosphere are CO, PH_3 and GeH_4. We have already seen that a sufficiently low oxygen abundance renders CO negligible while making PH_3 unconditionally stable, while the status of germane is essentially unaffected by the oxygen abundance. But what other species may plausibly be formed in greater quantities in a low-oxygen atmosphere than in a solar-composition gas? After N2 and ethane, are any of these species potential indicators of the oxygen content of the lower troposphere?

Of the many other organic species that are present in trace amounts at higher temperatures along the Jovian adiabat, methyl amine, ethylene, methyl mercaptan and HCN are the only species that even remotely approach ethane in abundance. Near 1200K all of these species have about 1% of the abundance of ethane (~0.1 ppb vs. 10 ppb for ethane). These levels are far too low for spectroscopic detection of ethylene, methyl amine and methyl mercaptan, which are subject to overwhelming interference from methane, ethane and NH3. Further, photochemical production of ethylene and methyl amine may mask such a deep-mixing source, and photochemical destruction of methyl mercaptan, CH3SH, should be rapid. The spectroscopic detection limit for HCN is on the order of 1 ppb, and indeed its detection in the upper troposphere has been reported (Tokunaga, et al., 1980). Within the uncertainty of our knowledge of the elemental abundances, thermal structure, and kinetic behavior of the atmosphere, we conclude that it is conceivable that the observed HCN originates from quenching of deep tropospheric gases by rapid convective overturn.

Effects of Lightning Discharges

The importance of electrical discharge activity on Jupiter has long been a matter of debate. Bar-Nun (1975) advocated an enormous rate of dissipation of energy by Jovian lightning, equivalent to at least the entire internal heat flux of the planet. Lewis (1976) argued that the efficiency of conversion of the total convective heat flux into lightning certainly could not reasonably be greater than unity. He advocated the use of the terrestrial conversion efficiency, about 10^{-4}, in the absence of any direct evidence for lightning on Jupiter. Calculations of the chemical effects of this amount of lightning on the atmosphere near the water cloud layer showed that the most abundant lightning-produced species in a solar-composition gas, CO, could not be produced in sufficient quantity to provide the observed amount of CO. These calculations also showed that that only very small concentrations of CO (2×10^{-14}), N_2 (2×10^{-15}), HCN (3×10^{-16}) and C_2H_2 (1×10^{-16}) would be found mixed into the bulk atmosphere (Lewis, 1980a). No other shock wave product would have a mole fraction higher than 10^{-17}.

Bar-Nun has continued to advocate enormous conversion efficiencies, and has claimed that lightning must be localized in the topmost (ammonia) cloud layer where the yields of organic products from shock events are much higher than in a solar-composition gas (where O is more abundant than C, and CO forms in preference to organic matter). However, the Voyager detection of lightning flashes and whistlers permits the conclusion that high-altitude lightning is several orders of magnitude rarer than Bar-Nun claims (Lewis, 1980b). A careful assessment of the total body of evidence regarding Jovian lightning (Borucki, et al., 1982) has led to the conclusion that the conversion efficiency of atmospheric convective energy flux into lightning is between 0.27×10^{-4} and 0.5×10^{-4}, in excellent agreement with the prejudices of Lewis (1976).

Because the relative importance of CO and organic compounds is a sensitive function of the C:O ratio, and because all of the models explored herein have C:O ratios greater than unity, it is clearly important to explore the consequences of lightning activity in these models. Note that, since C:O is everywhere greater than unity, there is no longer a fundamental distinction between the chemical consequences of high-altitude and low-altitude discharges.

We present first the mole fractions of a number of distinctive shock products in the shocked gas at a temperature of 2000K for the cases of:

1. O depleted 10x; peak shock pressure 50 b
2. O depleted 100x; peak shock pressure 50 b
3. O depleted 10x; peak shock pressure 10 b
4. O depleted 100x; peak shock pressure 10 b.

The graphite activity is indicated for each run: the abundances of organic compounds generally reach a maximum where the activity of graphite approaches unity. Note the great insensitivity of the the results to the degree of depletion of O once O is significantly less abundant than C. The bottom line in Table I gives the percent of total carbon converted into organic matter. The two 10-bar examples feature 33 and 35% conversion: it is obvious that no process whatsoever can be more than three times as efficient as this, no matter what assumptions are made!

Also note that the graphite activity reaches 0.7 in the latter runs. The highest possible value for the graphite activity, and hence for the abundances of carbon compounds, occurs almost exactly at the 2000K, 10 bar point illustrated. Under no circumstances can the activity of graphite surpass 1.000.

Several organic compounds, notably C2H2, HCN and C2H4, attain mole fractions greater than 10^-5 in the shocked gas. The total mole fraction of all organic species approaches 6.5x10^-4. The total yield of organic compounds thus can be as high as about 30 times the yield of organics in a shocked solar composition gas, in which the favored high-temperature carbon compound is CO.

Table I

Mole Fractions of Gases Shocked to 2000K

vs. (O depletion factor, shock pressure)

Species	(10x, 50b)	(100x, 50b)	(10x, 10b)	(100x, 10b)
CO	1.15×10^{-4}	1.16×10^{-5}	1.19×10^{-4}	1.19×10^{-5}
N_2	1.82×10^{-4}	1.82×10^{-4}	1.48×10^{-4}	1.46×10^{-4}
HCN	3.74×10^{-5}	3.85×10^{-5}	1.16×10^{-4}	1.18×10^{-4}
C_2H_2	3.73×10^{-5}	3.98×10^{-5}	4.41×10^{-4}	4.69×10^{-4}
C_2H_4	1.73×10^{-5}	1.84×10^{-5}	4.09×10^{-5}	4.31×10^{-5}
C_2H_6	4.75×10^{-7}	5.07×10^{-7}	2.25×10^{-7}	2.37×10^{-7}
CH_3CN	2.17×10^{-8}	2.31×10^{-8}	4.62×10^{-8}	4.85×10^{-8}
HCHO	5.25×10^{-9}	5.25×10^{-10}	1.08×10^{-9}	1.08×10^{-10}
CH_3NH_2	3.22×10^{-10}	3.22×10^{-10}	4.00×10^{-11}	4.09×10^{-11}
CH_3SH	1.67×10^{-10}	1.72×10^{-10}	1.11×10^{-10}	1.14×10^{-10}
CH_3OH	2.47×10^{-10}	2.47×10^{-11}	1.01×10^{-12}	1.01×10^{-13}
CO_2	8.72×10^{-11}	8.45×10^{-13}	5.32×10^{-12}	5.19×10^{-14}
a(graphite)	0.202	0.208	0.692	0.710
% C converted	5	5	33	35

Obviously, when the oxygen abundance is insufficient to use up more than a small portion of the available carbon, other compounds must be formed from that carbon. Since the only available elements with abundances greater than or comparable to C are H and N, obviously the compounds formed must be hydrocarbons, nitriles, amines, etc. The hydrocarbon abundances are enhanced by about a factor of 100, and HCN is enriched by about a factor of 10, in the O-depleted gas. However, it is important to realize that the 2-fold enrichment of N and the 5-fold enrichment of C assumed in these calculations account for an enrichment of C2 hydrocarbons by a factor of 25 and HCN by a factor of 10. Thus for the heavier hydrocarbons the effects of C enrichment and O depletion are comparable.

It is not sufficient simply to know how much of these products are present in the shocked gas. What we need to know is the over-all concentration of these species in the bulk atmosphere after quenching and mixing of the shocked gas with the unheated background gas. The method of calculation of Lewis (1980), modified to take into account the best available estimates of the lightning energy dissipation rate (Borucki, et al., 1982) will be used.

Borucki, et al., find that the rate of energy dissipation by Jovian lightning is about 0.36 erg/cm^2 s. We shall assume that this entire energy flux is employed in heating parcels of the Jovian atmosphere to exactly the optimum pressure and temperature conditions for synthesis of organic matter. Too low a shock temperature produces too little of the organic products, while shocking to too high a temperature wastes energy without increasing the yield of interestirg products. The 10-bar points in Table I are very close to that optimum. The energetic cost of heating the parcel to the optimum temperature (2000 to 2500K) is about 3×10^{11} erg/g. Thus the available lightning energy flux can shock about 1.2×10^{-12} g/cm^2 s to these optimum conditions. The total mass flux through the region of the water clouds is given by the product of the density times the mean vertical overturn speed, v. But v is just the ratio of the eddy diffusion coefficient K to the scale height H. For $K = 3\times10^8$, $H = 5\times10^6$, and a density of 10^{-4} g/cm^3, we calculate a turbulent mass flux of 8×10^{-3} g/cm^2 s through this region. The mass fraction of shocked gas in the total flow is then 1.5×10^{-10}. Thus a species produced with a mole fraction of 10^{-4} in the shocked gas (for example, HCN) would have a mole fraction of $\sim10^{-14}$ in the bulk atmosphere.

Table II summarizes the mole fractions of lightning-produced gases after dilution by turbulent mixing with the unshocked background atmosphere. In several ways, this is a generous estimate. First, the largest plausible enrichment factors for C and N are used. Second, water is assumed to be depleted to much less than the C abundance. Third, the very low-pressure conditions used tend to maximize the yield of organic matter per erg, but realistic shock events near the water saturation level on Jupiter (200 to 280K for the range of water abundances from 10^{-5} of solar to solar) will more typically run between 15 and 50 bars. At such high pressures the optimum conditions for formation of organic matter occur at much higher temperatures, and the

Table II

Mole Fractions of Lightning-Produced Gases

after mixing with Unshocked Atmosphere

C_2H_2	7.0×10^{-14}
N_2	2.7×10^{-14}
HCN	1.8×10^{-14}
C_2H_4	6.4×10^{-15}
C_2H_6	3.7×10^{-17}
CH_3CN	7.3×10^{-18}
CH_3SH	1.7×10^{-20}

energetic cost of achieving these higher temperatures will decrease the net energetic efficiency of the process. This will of course result in lower mole fractions of the products in the bulk atmosphere after dilution.

One cannot simply postulate that all lightning occurs at the ammonia cloud layer and therefore gives vastly better yields: in fact, the Voyager optical flash data place very severe limits on such flashes, and the very best of them would be only about twice as efficient in generating organic matter as the examples used in Table II. The main advantage of postulating such lightning is that the production of organic matter may be assigned to a region where the eddy mixing rate is low (say, 10^6 cm^2/s), and may thus result in greatly enhanced abundances of products. However, this is the logical equivalent of postulating extensive lightning at the tropopause on Earth. Such lightning is of course very rare, and is invariably associated with massive, highly turbulent nimbus towers that are so buoyant (due to latent heat release) that they penetrate and overshoot the tropopause. On Jupiter this kind of behavior would be ruled out on energetic grounds by a low water vapor abundance: if the requisite amount of water were present (perhaps 10 times the solar abundance), and if these motions remained coherent from the saturation lever (~300K) to the tropopause (~130K) over a vertical travel of 80 km, then the lightning products would be those for a wet atmosphere, rich in CO.

The observational implications of this discussion are easy to express: lightning discharges on Jupiter do not produce any products in observable amounts. So far as we can address the HCN abundance problem, the best available source appears to be quenching of hot gases at equilibrium near the 1200 to 1400K level along a Jovian adiabat.

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APPENDICES

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1 REM '       PROGRAM JUPITER
10 READ ABH, ABHE, ABO, ABC, ABN, ABSU, ABNE
20 FOR NT = 1 TO 10
22 INPUT "Temperature = ", TR
25 READ T, KH, KH2O, KCO, KCH4, KCO2
26 READ T, KOH, KO, KC, KH2S, KHS
27 READ T, KCN, KHCN, KNH3, KSO2, KS
28 READ T, KC2H6, KC2H4, KC2H2, KC3H8
29 READ T, KCH3OH, KHCHO, KHCOOH, KCH3SH
30 READ T, KCH3NH2, KCH3CN, KC2N2, KN2H4, KN
36 IF TR = T THEN 40 ELSE 25
40 INPUT "Use adiabat (1) or insert pressures (2)"; I
41 IF I = 1 THEN 45 ELSE 50
45 PR = 4.2E-08*T^3.33333
46 GOTO 60
50 INPUT "Total pressure (bars) = ",PR
60 ABH = .001*PR*ABH
61 ABHE = .001*ABHE*PR
62 ABO = .001*ABO*PR
63 ABC = .001*ABC*PR
64 ABN = .001*ABN*PR
65 ABSU = .001*ABSU*PR
66 ABNE = .001*ABNE*PR
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*KH2O*RH^2)
84 PH2 = RH^2
85 GR = ABC/((KCO*RO)+(KCH4*PH2^2))
86 RS = ABSU/((KSO2*RO^2)+(KH2S*PH2))
99 INDEX = 0
200 FOR ITER = 1 TO 100
201 INDEX = INDEX+1
202 PH = KH*RH
203 PH2 = RH^2
204 PHE = ABHE
205 PNE = ABNE
210 PCO = KCO*GR*RO
211 PCH4 = KCH4*GR*PH2^2
212 PCO2 = KCO2*GR*RO^2
213 PC = KC*GR
214 PC2H6 = KC2H6*PH2^3*GR^2
215 PC2H4 = KC2H4*PH2^2*GR^2
216 PC2H2 = KC2H2*PH2*GR^2
217 PC3H8 = KC3H8*PH2^4*GR^3
220 POH = KOH*RH*RO
221 PH2O = KH2O*PH2*RO
222 PO = KO*RO
223 PO2 = RO^2
224 PCH3OH = KCH3OH*GR*RO*PH2^2
225 PHCHO = KHCHO*GR*RO*PH2
226 PHCOOH = KHCOOH*GR*PO2*PH2
230 PCN = KCN*GR*RN
231 PHCN = KHCN*GR*RH*RN
232 PNH3 = KNH3*RN*PH2*RH
233 PN2 = RN^2
234 PN = RN*KN
235 PC2N2 = KC2N2*PN2*GR^2
236 PCH3CN = KCH3CN*RN*RH*PH2*GR^2
237 PN2H4 = KN2H4*PN2*PH2^2
238 PCH3NH2 = KCH3NH2*GR*RN*RH*PH2^2
240 PH2S = KH2S*RS*PH2
241 PSO2 = KSO2*RS*PO2
242 PHS = KHS*RH*RS
```

```
243 PS = KS*RS
244 PS2 = RS^2
245 PCH3SH = KCH3SH*GR*RS*PH2^2
400 REM CALCULATE ELEMENTAL SUMS
401 SH = (PH+POH+PHS+PHCN)+2*(PH2+PH2O+PH2S+PC2H2+PHCHO+PHCOOH)+3*(PCH3CN+PNH3)+
4*(PC2H4+PCH3OH+PCH3SH+PN2H4+PCH4)+5*PCH3NH2+6*PC2H6
402 SC = PCO+PCO2+PCH4+PC+PHCN+PCN+PCH3OH+PHCHO+PHCOOH+PCH3NH2+PCH3SH+2*(PC2H2+P
C2H4+PC2H6+PCH3CN+PC2N2)
403 SO = PH2O+PCO+POH+PO+PCH3OH+PCH3OH+2*(PO2+PCO2+PSO2+PHCOOH)
404 SN = PN+PNH3+PCN+PHCN+PCH3NH2+PCH3CN+2*(PN2+PC2N2+PN2H4)
405 SS = PS+PHS+PSO2+PH2S+PCH3SH+2*PS2
419 P = PH2+PH+PH2O+PCO+PCO2+PCH4+PN2+PNH3+POH+PH2S+PHE+PO+PNE+PHS
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-ABSU)/ABSU
440 IF EH<.001 THEN IF EO<.001 THEN IF EC<.001 THEN IF EN<.001 THEN IF ES<.001 T
HEN GOTO 501 ELSE GOTO 449
449 REM COMPARE ELEMENTAL SUMS TO ABUNDANCES
450 IF INDEX = 1 THEN 452
451 GOTO 455
452 RH = RH*SQR(ABH/SH)
453 GOTO 500
455 IF INDEX = 2 THEN 457
456 GOTO 460
457 RO = RO*(ABO/SO)
458 GOTO 500
460 IF INDEX = 3 THEN 462
461 GOTO 465
462 GR = GR*(ABC/SC)
463 GOTO 500
465 IF INDEX = 4 THEN 467
466 GOTO 470
467 RN = RN*SQR(ABN/SN)
468 GOTO 500
470 IF INDEX = 5 THEN 472
471 GOTO 488
472 RS = RS*(ABSU/SS)
488 INDEX = 0
500 NEXT ITER
501 REM OUTPUT RESULTS OF ITERATION
502 PLAY "mlt22002c8d8e8f8g8a8b803c202b16a16g16f16e16d16c2"
505 PRINT "Temperature = ";T, "Pressure = ";P;"bars    ";ITER;"iterations"
506 PRINT
507 PRINT "                    Pressures of gases in bars"
508 PRINT "H =";PH;" H2 =";PH2;" He =";PHE;" Ne =";PNE
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
512 PRINT "S =";PS;" S2 =";PS2;" HS =";PHS;" H2S =";PH2S
513 PRINT "C2H6 = ";PC2H6;" C2H4 = ";PC2H4;" C2H2 = ";PC2H2
514 PRINT "CH3OH = ";PCH3OH;" HCHO = ";PHCHO;" HCOOH = ";PHCOOH
515 PRINT "CH3NH2 = ";PCH3NH2;" CH3CN = ";PCH3CN;" C2N2 = ";PC2N2
516 PRINT "N2H4 = ";PN2H4;" HCN = ";PHCN;" CH3SH = ";PCH3SH;" SO2 = ";PSO2
519 PRINT
520 PRINT "INPUT ABUNDANCES OF ELEMENTS"
521 PRINT "H =";ABH;" O =";ABO;" C =";ABC;" N =";ABN;" S =";ABSU
522 PRINT "                                        Graphite activity ="; GR
523 PRINT "CALCULATED ABUNDANCES OF ELEMENTS
524 PRINT "H =";SH;" O =";SO;" C =";SC;" N =";SN;" S =";SS
545 INPUT "Type 1 to continue, 0 to end:", GOON
546 IF GOON = 1 THEN 600
547 GOTO 3000
600 NEXT NT
1000 DATA 1756,122.,1.192,.6516,0.2065,0.0221,0.2295
```

```
1201 DATA 2000, 1.622E-3, 3467.4, 2.944E7, 3.908E-4, 2.254E10
1202 DATA 2000, 0.5808, 6.637E-4, 3.342E-11, 0.614, 0.1033
1203 DATA 2000, 2.183E-7, 1.472E-2, 2.046E-5, 4.498E5, 2.891E-3
1204 DATA 2000, 7.063E-9, 1.121E-5, 1.054E-3, 1.033E-13
1205 DATA 2000, 3.289E-3, 30.52, 3.674E4, 5.408E-7
1206 DATA 2000, 6.683E-11, 9.736E-7, 1.647E-6, 5.768E-15, 9.5E-10
1211 DATA 1900, 7.907E-4, 7691, 4.275E7, 5.236E-4, 7.907 E10
1212 DATA 1900, 1.932, 2.958E-4, 3.467E-12, .817, 4.2E-2
1213 DATA 1900, 1.972E-07, 9.705E-3, 2.438E-5, 1.406E6, 1.442E-3
1214 DATA 1900, 9.496E-9, 9.669E-6, 5.164E-4, 1.484E-13
1215 DATA 1900, 6.349E-3, 44.51, 1.230E5, 7.412E-6
1216 DATA 1900, 7.366E-11, 7.470E-7, 6.166E-7, 4.328E-15, 9.496E-9
1221 DATA 1800, 3.565E-4, 1.862E4, 6.471E7, 1.342E-3, 3.192E11
1222 DATA 1800, 2.203, 1.005E-4, 2.805E-13, 1.122, 3.147E-2
1223 DATA 1800, 4.345E-8, 9.462E-3, 2.965E-5, 5E6, 6.653E-4
1224 DATA 1800, 1.318E-8, 8.204E-6, 2.333E-4, 2.223E-13
1225 DATA 1800, 1.318E-2, 67.70, 4.712E5, 1.052E-5
1226 DATA 1800, 8.204E-11, 5.559E-7, 2.070E-7, 3.148E-15, 3.656E-11
1251 DATA 1500, 1.754E-5, 5.309E5, 3.054E8, 2.630E-3, 6.324E13
1252 DATA 1500, 3.622, 4.037E-6, 1.949E-17, 3.758, 1.1E-2
1253 DATA 1500, 1.368E-10, 1.663E-3, 6.252E-3, 6.237E8, 3.556E-5
1254 DATA 1500, 4.592E-8, 4.387E-6, 1.141E-5, 1.031E-12
1255 DATA 1500, .2110, 3.332E2,  7.757E7, 3.984E-5
1256 DATA 1500, 1.231E-10, 1.817E-7, 3.265E-9, 9.354E-16, 6.067E-14
1281 DATA 1200, 1.963E-7, 7.925E7, 3.013E9, 1.581E-2, 1.750E17
1282 DATA 1200, 7.709, 2.489E-8, 1.114E-23, 23.12, 2.198E-3
1283 DATA 1200, 2.339E-14, 1.227E-4, 1.923E-4, 8.77E11, 4.446E-7
1284 DATA 1200, 2.992E-7, 1.721E-6, 1.234E-7, 1.029E-11
1285 DATA 1200, 13.59, 3.637E3, 1.638E11, 2.935E-4
1286 DATA 1200, 2.265E-10, 3.390E-8, 6.470E-13, 1.517E-16, 4.197E-18
1301 DATA 1000, 2.259E-9, 1.153E10, 2.877E10, 9.75E-2, 4.786E20
1302 DATA 1000, 16.51, 1.56E-10, 6.31E-30, 141.6, 4.457E-4
1303 DATA 1000, 3.9E-18, 9.036E-6, 5.848E-4, 1.245E15, 5.623E-9
1304 DATA 1000, 1.945E-6, 6.714E-7, 1.334E-10, 1.028E-10
1305 DATA 1000, 873., 3.972E4, 3.459E14, 2.163E-3
1306 DATA 1000, 4.169E-10, 6.324E-9, 1.282E-14, 2.46E-17, 2.965E-22
1321 DATA  800, 2.891E-12, 1.945E13, 8.204E11, 1.4, 6.761E25
1322 DATA  800, 52.481, 7.925E-14, 0, 2.099E3, 4.0467E-5
1323 DATA  800, 8.166E-24, 1.853E-7, 2.999E-3, 6.683E19, 8.185E-12
1324 DATA  800, 3.228E-5, 2.042E-7, 1.603E-12, 4.808E-9
1325 DATA  800, 5.794E5, 1.66E6, 3.767E19, 4.325E-2
1326 DATA  800, 1.361E-9, 6.012E-10, 1.081E-18, 1.82E-18, 1.803E-28
1341 DATA  600, 4.613E-17, 4.295E18, 2.08E14, 100.2, 2.541E34
1342 DATA  600, 367.3, 2.667E-19, 0, 4887., 2.004E-8
1343 DATA  600, 2.71E-33, 2.786E-10, 4.169E-2, 1.406E26, 4.335E-18
1344 DATA  600, 3.485E-3, 2.404E-8, 2.028E-7, 2.168E-6
1345 DATA  600, 2.449E10, 7.464E8, 8.670E27, .153
1346 DATA  600, 8.222E-9, 1.057E-11, 1.791E-24, 2.228E-20, 8.298E-39
3000 END
```

Appendix 2


```
Ok
RUN
Temperature = 2000
Use adiabat (1) or insert pressures (2)? 1
Temperature =  2000          Pressure =  4231.117 bars     55 iterations

                  Pressures of gases in bars
H = 9.872717E-02  H2 = 3704.859  He = 516.4525  Ne = .9715232
O = 2.603932E-10  O2 = 1.539273E-13  OH = 1.38698E-05  H2O = 5.040033
N = 1.672887E-10  N2 = 3.100888E-02  NH3 = .8124676  CN = 1.972217E-11
C = 1.714606E-14  CO = 5.925889E-03  CO2 = 1.78003E-06  CH4 = 2.752047
S = 1.18569E-07  S2 = 1.682077E-09  HS = 2.578749E-04  H2S = 9.329599E-02
C2H6 =  9.454096E-05  C2H4 =  4.050091E-05  C2H2 =  1.027846E-06
CH3OH =  9.087049E-06  HCHO =  2.275998E-05  HCOOH =  1.07494E-08
CH3NH2 =  5.044307E-06  CH3CN =  1.017646E-08  C2N2 =  1.344298E-14
N2H4 =  2.455018E-09  HCN =  8.094584E-05  CH3SH =  1.561928E-07  SO2 =
 2.839605E-12

INPUT ABUNDANCES OF ELEMENTS
H = 7433.529  O = 5.045995  C = 2.758364  N = .8741592  S = 9.355409E-02
                                    Graphite activity = 5.130479E-04
CALCULATED ABUNDANCES OF ELEMENTS
H = 7433.529  O = 5.045994  C = 2.758365  N = .8745714  S = 9.355414E-02
Type 1 to continue, 0 to end:
1LIST   2RUN   3LOAD"  4SAVE"  5CONT 6,"LPT1 7TRON 8TROFF9KEY    0SCREEN

Ok
RUN
Temperature = 1900
Use adiabat (1) or insert pressures (2)? 1
Temperature =  1900          Pressure =  3566.139 bars     55 iterations

                  Pressures of gases in bars
H = 4.418467E-02  H2 = 3122.624  He = 435.2879  Ne = .8188406
O = 5.234005E-11  O2 = 3.13092E-14  OH = 1.910306E-05  H2O = 4.249506
N = 1.529486E-09  N2 = 2.594236E-02  NH3 = .685201  CN = 1.444064E-11
C = 1.576262E-15  CO = 3.439115E-03  CO2 = 1.125533E-06  CH4 = 2.321206
S = 4.452742E-08  S2 = 9.535084E-10  HS = 7.247219E-05  H2S = 7.877784E-02
C2H6 =  5.97653E-05  C2H4 =  1.948814E-05  C2H2 =  3.333153E-07
CH3OH =  4.980299E-06  HCHO =  1.118119E-05  HCOOH =  5.467281E-09
CH3NH2 =  2.939073E-06  CH3CN =  4.339645E-09  C2N2 =  3.306453E-15
N2H4 =  1.094804E-09  HCN =  3.971319E-05  CH3SH =  1.014639E-06  SO2 =
 1.359313E-12

INPUT ABUNDANCES OF ELEMENTS
H = 6265.291  O = 4.252977  C = 2.324865  N = .7367782  S = 7.885133E-02
                                    Graphite activity = 4.546474E-04
CALCULATED ABUNDANCES OF ELEMENTS
H = 6265.291  O = 4.252976  C = 2.324865  N = .7371283  S = 7.885136E-02
Type 1 to continue, 0 to end:
1LIST   2RUN   3LOAD"  4SAVE"  5CONT 6,"LPT1 7TRON 8TROFF9KEY    0SCREEN
```

```
Ok
RUN
Temperature = 1800
Use adiabat (1) or insert pressures (2)? 1
Temperature =  1800          Pressure =  2978.005 bars     55 iterations

                 Pressures of gases in bars
H = 1.820473E-02  H2 = 2607.649  He = 363.5012  Ne = .6837993
O = 7.349113E-12  O2 = 5.34734E-15  OH = 8.226365E-06  H2O = 3.550567
N = 5.309413E-12  N2 = .0210902  NH3 = .573375  CN = 1.341747E-12
C = 5.964491E-17  CO = 1.006192E-03  CO2 = 3.629453E-07  CH4 = 1.9404
S = 1.496487E-08  S2 = 5.059538E-10  HS = 3.614738E-05  H2S = 6.581084E-02
C2H6 =  1.056681E-05  C2H4 =  2.522348E-06  C2H2 =  2.750711E-08
CH3OH =  1.393552E-06  HCHO =  2.745031E-06  HCOOH =  1.397117E-09
CH3NH2 =  8.796895E-07  CH3CN =  4.860623E-10  C2N2 =  1.973932E-16
N2H4 =  4.514542E-10  HCN =  1.492067E-05  CH3SH =  3.421448E-07  SO2 =
 6.013996E-13

INPUT ABUNDANCES OF ELEMENTS
H = 5232.033  O = 3.551585  C = 1.941454  N = .6152704  S = 6.584734E-02
                              Graphite activity = 2.126379E-04
CALCULATED ABUNDANCES OF ELEMENTS
H = 5232.031  O = 3.551585  C = 1.941454  N = .6155712  S = 6.584735E-02
Type 1 to continue, 0 to end:
1LIST   2RUN  3LOAD"  4SAVE"  5CONT 6,"LPT1 7TRON 8TROFF9KEY    0SCREEN

Ok
RUN
Temperature = 1500
Use adiabat (1) or insert pressures (2)? 1
Temperature =  1500          Pressure =  1621.74 bars     70 iterations

                 Pressures of gases in bars
H = 6.609692E-04  H2 = 1420.049  He = 197.9564  Ne = .3723851
O = 1.035603E-14  O2 = 6.580658E-18  OH = 3.501344E-07  H2O = 1.933974
N = 6.079574E-17  N2 = 1.004149E-06  NH3 = .3352532  CN = 2.732402E-17
C = 3.884924E-21  CO = 1.561576E-04  CO2 = 8.295081E-08  CH4 = 1.057113
S = 2.389296E-10  S2 = 4.514545E-11  HS = 2.785168E-06  H2S = 3.585643E-02
C2H6 =  5.224327E-06  C2H4 =  3.514738E-07  C2H2 =  6.43736E-10
CH3OH =  2.17562E-07  HCHO =  2.41937E-07  HCOOH =  1.44486E-10
CH3NH2 =  1.868421E-09  CH3CN =  3.871041E-13  C2N2 =  1.302568E-22
N2H4 =  1.894096E-15  HCN =  1.251706E-08  CH3SH =  1.07595E-07  SO2 =
 2.757732E-14

INPUT ABUNDANCES OF ELEMENTS
H = 2849.273  O = 1.934131  C = 1.057282  N = .3350654  S = 3.585931E-02
                              Graphite activity = 1.993239E-04
CALCULATED ABUNDANCES OF ELEMENTS
H = 2849.272  O = 1.934131  C = 1.057282  N = .3352552  S = 3.585932E-02
Type 1 to continue, 0 to end:
1LIST   2RUN  3LOAD"  4SAVE"  5CONT 6,"LPT1 7TRON 8TROFF9KEY    0SCREEN
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OK
RUN
Temperature = 1200
Use adiabat (1) or insert pressures (2)? 1
Temperature =  1200           Pressure =  770.8155 bars     60 iterations

                    Pressures of gases in bars
H = 5.09985E-06  H2 = 674.954  He = 94.08841  Ne = .1769942
O = 4.277621E-19  O2 = 2.953622E-22  OH = 3.442014E-09  H2O = .9192864
N = 1.930491E-19  N2 = 2.115718E-03  NH3 = .1551027  CN = 7.506413E-20
C = 7.772461E-28  CO = 3.61285E-06  CO2 = 3.606337E-09  CH4 = .5025201
S = 4.855953E-13  S2 = 1.192916E-12  HS = 6.236913E-08  H2S = 1.704382E-02
C2H6 =  4.47848E-07  C2H4 =  3.816592E-09  C2H2 =  4.054488E-13
CH3OH =  7.423667E-09  HCHO =  2.943528E-09  HCOOH =  2.278328E-12
CH3NH2 =  8.603116E-09  CH3CN =  1.331026E-13  C2N2 =  6.663599E-24
N2H4 =  1.462149E-13  HCN =  1.023019E-08  CH3SH =  1.018907E-08  SO2 =
 2.829173E-16

INPUT ABUNDANCES OF ELEMENTS
H = 1354.256  O = .9192901  C = .5025246  N = .1592562  S = 1.704388E-02
                                      Graphite activity = 6.977075E-05
CALCULATED ABUNDANCES OF ELEMENTS
H = 1354.256  O = .9192901  C = .5025246  N = .1593342  S = 1.704389E-02
Type 1 to continue, 0 to end:
1LIST   2RUN   3LOAD"  4SAVE"  5CONT 6,"LPT1 7TRON 8TROFF9KEY    0SCREEN

Ok
RUN
Temperature = 1000
Use adiabat (1) or insert pressures (2)? 1
Temperature =  1000           Pressure =  419.7687 bars     60 iterations

                    Pressures of gases in bars
H = 4.330945E-08  H2 = 367.5638  He = 51.23862  Ne = .0963874
O = 1.842793E-23  O2 = 1.395416E-26  OH = 3.739084E-11  H2O = .5006265
N = 6.181932E-24  N2 = 4.347094E-04  NH3 = 8.592231E-02  CN = 1.689322E-24
C = 1.310925E-34  CO = 7.060576E-08  CO2 = 1.387474E-10  CH4 = .2736645
S = 1.002772E-15  S2 = 3.180299E-14  HS = 1.523853E-09  H2S = 9.281751E-03
C2H6 =  4.168833E-08  C2H4 =  3.915106E-11  C2H2 =  2.11634E-17
CH3OH =  2.894542E-10  HCHO =  3.582961E-11  HCOOH =  3.68583E-14
CH3NH2 =  4.677476E-10  CH3CN =  4.010396E-16  C2N2 =  2.405381E-27
N2H4 =  1.444773E-15  HCN =  7.50396E-11  CH3SH =  1.08269E-09  SO2 =
 3.098182E-18

INPUT ABUNDANCES OF ELEMENTS
H = 737.5001  O = .5006266  C = .2736646  N = 8.672766E-02  S = 9.28175E-03
                                      Graphite activity = 2.077535E-05
CALCULATED ABUNDANCES OF ELEMENTS
H = 737.4998  O = .5006266  C = .2736646  N = 8.679173E-02  S = 9.281754E-03
Type 1 to continue, 0 to end:
1LIST   2RUN   3LOAD"  4SAVE"  5CONT 6,"LPT1 7TRON 8TROFF9KEY    0SCREEN
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Ok
RUN
Temperature = 800
Use adiabat (1) or insert pressures (2)? 1
Temperature =  800           Pressure =  199.5163 bars     65 iterations

                   Pressures of gases in bars
H = 3.821188E-11  H2 = 174.7031  He = 24.35378  Ne = 4.581306E-02
O = 5.549603E-30  O2 = 4.903715E-33  OH = 4.857525E-14  H2O = .2379484
N = 1.071984E-30  N2 = 3.534962E-05  NH3 = 4.117369E-02  CN = 1.477951E-31
C = 0  CO = 1.748826E-10  CO2 = 1.00924E-12  CH4 = .1300732
S = 9.847014E-20  S2 = 1.447344E-16  HS = 6.434833E-12  H2S = 4.411629E-03
C2H6 =  1.594969E-09  C2H4 =  5.775289E-14  C2H2 =  2.595081E-21
CH3OH =  3.769647E-12  HCHO =  6.182015E-14  HCOOH =  9.823807E-17
CH3NH2 =  9.937118E-12  CH3CN =  7.648546E-20  C2N2 =  3.54101E-34
N2H4 =  1.96362E-18  HCN =  4.432783E-14  CH3SH =  4.834278E-11  SO2 =
 3.942599E-21

INPUT ABUNDANCES OF ELEMENTS
H = 350.5348  O = .2379484  C = .1300732  N = 4.122177E-02  S = 4.411628E-03
                                     Graphite activity = 3.044096E-06
CALCULATED ABUNDANCES OF ELEMENTS
H = 350.5348  O = .2379484  C = .1300732  N = 4.124439E-02  S = 4.411629E-03
Type 1 to continue, 0 to end:
1LIST   2RUN   3LOAD"   4SAVE"   5CONT 6,"LPT1 7TRON 8TROFF9KEY    0SCREEN

RUN
Temperature = 600
Use adiabat (1) or insert pressures (2)? 1
Temperature =  600           Pressure =  76.47441 bars     65 iterations

                   Pressures of gases in bars
H = 3.774874E-16  H2 = 66.9635  He = 9.334786  Ne = 1.756011E-02
O = 0  O2 = 0  OH = 9.531462E-19  H2O = 9.120545E-02
N = 0  N2 = 4.791225E-07  NH3 = 1.581293E-02  CN = 0
C = 0  CO = 7.319215E-15  CO2 = 0  CH4 = 4.985694E-02
S = 2.239988E-26  S2 = 2.670011E-17  HS = 8.473705E-16  H2S = 1.690974E-03
C2H6 =  1.288488E-11  C2H4 =  1.327315E-18  C2H2 =  1.672128E-19
CH3OH =  3.864259E-15  HCHO =  1.758778E-18  HCOOH =  0
CH3NH2 =  2.317276E-14  CH3CN =  4.936496E-26  C2N2 =  0
N2H4 =  4.786719E-23  HCN =  1.751077E-19  CH3SH =  3.933742E-13  SO2 =  0

INPUT ABUNDANCES OF ELEMENTS
H = 134.3597  O = 9.120545E-02  C = 4.985694E-02  N = 1.580027E-02  S =
 1.690973E-03
                                     Graphite activity = 1.109639E-07
CALCULATED ABUNDANCES OF ELEMENTS
H = 134.3597  O = 9.120545E-02  C = 4.985694E-02  N = 1.581389E-02  S =
 1.690974E-03
Type 1 to continue, 0 to end:
1LIST   2RUN   3LOAD"   4SAVE"   5CONT 6,"LPT1 7TRON 8TROFF9KEY    0SCREEN
```

```
O depleted by 10x; 5x solar C; 2x solar N
Temperature =  2000          Pressure =  4219.798 bars      50 iterations

                   Pressures of gases in bars
H = 9.847902E-02  H2 = 3686.258  He = 516.4525  Ne = .9715232
O = 2.604543E-11  O2 = 1.539996E-15  OH = 1.383819E-06  H2O = .5015906
N = 3.166214E-10  N2 = .1110793  NH3 = 1.526163  CN = 1.888116E-10
C = 8.672909E-14  CO = 2.998167E-03  CO2 = 9.008069E-08  CH4 = 13.78111
S = 1.191657E-07  S2 = 1.69905E-09  HS = 2.585213E-04  H2S = 9.329476E-02
C2H6 =  2.382665E-03  C2H4 =  1.025873E-03  C2H2 =  2.616634E-05
CH3OH =  4.551488E-06  HCHO =  1.145746E-05  HCOOH =  5.41256E-10
CH3NH2 =  4.768817E-05  CH3CN =  4.89094E-07  C2N2 =  1.232093E-12
N2H4 =  8.706225E-09  HCN =  7.72993E-04  CH3SH =  7.860851E-07  SO2 =
 2.855236E-14

INPUT ABUNDANCES OF ELEMENTS
H = 7433.529  O = .5045995  C = 13.79182  N = 1.748319  S = 9.355409E-02
                                     Graphite activity = 2.595125E-03
CALCULATED ABUNDANCES OF ELEMENTS
H = 7433.527  O = .5045994  C = 13.79182  N = 1.749142  S = 9.355418E-02
Type 1 to continue, 0 to end:
Ok


1LIST   2RUN   3LOAD"   4SAVE"   5CONT 6,"LPT1 7TRON 8TROFF9KEY     0SCREEN

O depleted by 10x; 5x solar C; 2x solar N
Temperature =  1800          Pressure =  2970.04 bars      50 iterations

                   Pressures of gases in bars
H = 1.815896E-02  H2 = 2594.554  He = 363.5012  Ne = .6837993
O = 7.37766E-13  O2 = 5.388962E-17  OH = 8.237557E-07  H2O = .3546459
N = 1.006977E-11  N2 = 7.586244E-02  NH3 = 1.079275  CN = 1.285769E-11
C = 3.01365E-16  CO = 5.103685E-04  CO2 = 1.84811E-08  CH4 = 9.705944
S = 1.504007E-08  S2 = 5.110518E-10  HS = 3.62377E-05  H2S = 6.580941E-02
C2H6 =  2.657194E-04  C2H4 =  6.374863E-05  C2H2 =  6.987104E-07
CH3OH =  6.997667E-07  HCHO =  1.385364E-06  HCOOH =  7.078366E-11
CH3NH2 =  8.324452E-06  CH3CN =  2.335737E-08  C2N2 =  1.812662E-14
N2H4 =  1.607633E-09  HCN =  1.426224E-04  CH3SH =  1.72002E-06  SO2 =
 6.091266E-15

INPUT ABUNDANCES OF ELEMENTS
H = 5232.033  O = .3551585  C = 9.707269  N = 1.230541  S = 6.584734E-02
                                     Graphite activity = 1.074385E-03
CALCULATED ABUNDANCES OF ELEMENTS
H = 5232.031  O = .3551585  C = 9.707269  N = 1.231151  S = 6.584739E-02
Type 1 to continue, 0 to end:
Ok


1LIST   2RUN   3LOAD"   4SAVE"   5CONT 6,"LPT1 7TRON 8TROFF9KEY     0SCREEN
```

```
O depleted by 10x; 5x solar C; 2x solar N
Temperature =  1500          Pressure =  1617.344 bars      70 iterations

                     Pressures of gases in bars
H = 6.592866E-04  H2 = 1412.828  He = 197.9564  Ne = .3723851
O = 1.040552E-15  O2 = 6.643705E-20  OH = 3.509121E-08  H2O = .1933336
N = 1.22525E-16  N2 = 4.078506E-06  NH3 = .6705075  CN = 2.781847E-16
C = 1.962495E-20  CO = 7.926305E-05  CO2 = 4.230569E-09  CH4 = 5.286049
S = 2.401472E-10  S2 = 4.5607E-11  HS = 2.792243E-06  H2S = 3.585601E-02
C2H6 =  1.312996E-04  C2H4 =  8.8785E-06  C2H2 =  1.634437E-08
CH3OH =  1.093108E-07  HCHO =  1.221789E-07  HCOOH =  7.331453E-12
CH3NH2 =  1.878143E-08  CH3CN =  1.975754E-11  C2N2 =  1.350136E-20
N2H4 =  7.615127E-15  HCN =  1.271113E-07  CH3SH =  5.407673E-07  SO2 =
 2.798348E-16

INPUT ABUNDANCES OF ELEMENTS
H = 2849.273  O = .1934131  C = 5.286409  N = .6701309  S = 3.585931E-02
                                        Graphite activity = 1.006924E-03
CALCULATED ABUNDANCES OF ELEMENTS
H = 2849.272  O = .1934131  C = 5.286409  N = .6705157  S = 3.585934E-02
Type 1 to continue, 0 to end:
Ok


1LIST   2RUN   3LOAD"  4SAVE"  5CONT 6,"LPT1 7TRON 8TROFF9KEY    0SCREEN

O depleted by 10x; 5x solar C; 2x solar N
Temperature =  1200          Pressure =  768.7373 bars      55 iterations

                     Pressures of gases in bars
H = 5.086935E-06  H2 = 671.5398  He = 94.08841  Ne = .1769942
O = 4.2993E-20  O2 = 2.983635E-24  OH = 3.450697E-10  H2O = 9.192717E-02
N = 3.792444E-19  N2 = 8.16508E-03  NH3 = .3023898  CN = 7.448318E-19
C = 3.925844E-27  CO = 1.834086E-06  CO2 = 1.840058E-10  CH4 = 2.512599
S = 4.88063E-13  S2 = 1.205072E-12  HS = 6.252734E-08  H2S = 1.704378E-02
C2H6 =  1.125311E-05  C2H4 =  9.638732E-08  C2H2 =  1.029159E-11
CH3OH =  3.730642E-09  HCHO =  1.486742E-09  HCOOH =  1.156589E-13
CH3NH2 =  8.428991E-08  CH3CN =  6.620383E-12  C2N2 =  6.560852E-22
N2H4 =  5.585853E-13  HCN =  1.012531E-07  CH3SH =  5.120423E-08  SO2 =
 2.872445E-18

INPUT ABUNDANCES OF ELEMENTS
H = 1354.256  O = .091929  C = 2.512623  N = .3185124  S = 1.704388E-02
                                        Graphite activity = 3.524097E-04
CALCULATED ABUNDANCES OF ELEMENTS
H = 1354.255  O = .091929  C = 2.512623  N = .3187201  S = .0170439
Type 1 to continue, 0 to end:
Ok


1LIST   2RUN   3LOAD"  4SAVE"  5CONT 6,"LPT1 7TRON 8TROFF9KEY    0SCREEN
```

```
O'depleted by 10x; 5x solar C; 2x solar N
Temperature =  1000          Pressure =  418.6334 bars     60 iterations

                    Pressures of gases in bars
H = 4.319944E-08  H2 = 365.6989  He = 51.23862  Ne = .0963874
O = 1.852189E-24  O2 = 1.409682E-28  OH = 3.748603E-12  H2O = 5.006262E-02
N = 1.233176E-23  N2 = 1.72982E-03  NH3 = .1700957  CN = 1.702163E-23
C = 6.621639E-34  CO = 3.584567E-08  CO2 = 7.079948E-12  CH4 = 1.368321
S = 1.007885E-15  S2 = 3.212818E-14  HS = 1.527733E-09  H2S = 9.281751E-03
C2H6 =  1.047521E-06  C2H4 =  9.887828E-10  C2H2 =  5.372195E-16
CH3OH =  1.454649E-10  HCHO =  1.809796E-11  HCOOH =  1.871249E-15
CH3NH2 =  4.653476E-09  CH3CN =  2.025583E-14  C2N2 =  2.442087E-25
N2H4 =  5.690929E-15  HCN =  7.541793E-10  CH3SH =  5.441053E-09  SO2 =
 3.145818E-20

INPUT ABUNDANCES OF ELEMENTS
H = 737.5001  O = 5.006265E-02  C = 1.368323  N = .1734553  S = 9.28175E-03
                                       Graphite activity = 1.049388E-04
CALCULATED ABUNDANCES OF ELEMENTS
H = 737.5  O = 5.006266E-02  C = 1.368323  N = .1735553  S = 9.281758E-03
Type 1 to continue, 0 to end:
Ok


1LIST   2RUN  3LOAD"  4SAVE"  5CONT 6,"LPT1 7TRON 8TROFF9KEY    0SCREEN

Temperature =  800           Pressure =  198.9755 bars     60 iterations

                    Pressures of gases in bars
H = 3.811463E-11  H2 = 173.815  He = 24.35378  Ne = 4.581306E-02
O = 5.577958E-31  O2 = 4.953954E-35  OH = 4.869919E-15  H2O = 2.379484E-02
N = 2.157579E-30  N2 = 1.431997E-04  NH3 = 8.223911E-02  CN = 1.502573E-30
C = 0  CO = 8.878852E-11  CO2 = 5.150129E-14  CH4 = .6503657
S = 9.897338E-20  S2 = 1.462175E-16  HS = 6.451257E-12  H2S = 4.411633E-03
C2H6 =  4.007795E-08  C2H4 =  1.458614E-12  C2H2 =  6.587657E-20
CH3OH =  1.894454E-12  HCHO =  3.122673E-14  HCOOH =  4.987581E-18
CH3NH2 =  9.97476E-11  CH3CN =  3.897904E-18  C2N2 =  3.659975E-32
N2H4 =  7.873866E-18  HCN =  4.495161E-13  CH3SH =  2.429492E-10  SO2 =
 4.003347E-23

INPUT ABUNDANCES OF ELEMENTS
H = 350.5348  O = 2.379484E-02  C = .6503658  N = 8.244354E-02  S =
 4.411628E-03
                                       Graphite activity = 1.537642E-05
CALCULATED ABUNDANCES OF ELEMENTS
H = 350.5346  O = 2.379484E-02  C = .6503658  N = 8.252551E-02  S =
 4.411634E-03
Type 1 to continue, 0 to end:
Ok

1LIST   2RUN  3LOAD"  4SAVE"  5CONT 6,"LPT1 7TRON 8TROFF9KEY    0SCREEN
```

```
O depleted by 10x; 5x solar C; 2x solar N
Temperature =  600            Pressure =  76.26707 bars     65 iterations

                  Pressures of gases in bars
H = 3.765265E-16  H2 = 66.623  He = 9.334786  Ne = 1.756011E-02
O = 0  O2 = 0  OH = 9.555786E-20  H2O = 9.120545E-03
N = 0  N2 = 1.945733E-06  NH3 = 3.162349E-02  CN = 0
C = 0  CO = 3.716005E-15  CO2 = 0  CH4 = .2492847
S = 2.251438E-26  S2 = 2.697377E-17  HS = 8.495338E-16  H2S = 1.690976E-03
C2H6 =  3.237684E-10  C2H4 =  3.352293E-17  C2H2 =  4.244742E-18
CH3OH =  1.942004E-15  HCHO =  8.884006E-19  HCOOH =  0
CH3NH2 =  2.328944E-13  CH3CN =  2.518906E-24  C2N2 =  0
N2H4 =  1.924185E-22  HCN =  1.777929E-18  CH3SH =  1.976925E-12  SO2 =  0

INPUT ABUNDANCES OF ELEMENTS
H = 134.3597  O = 9.120544E-03  C = .2492847  N = 3.160054E-02  S =
 1.690973E-03
                                    Graphite activity = 5.605051E-07
CALCULATED ABUNDANCES OF ELEMENTS
H = 134.3596  O = 9.120545E-03  C = .2492847  N = 3.162738E-02  S =
 1.690976E-03
Type 1 to continue, 0 to end:
Ok

1LIST   2RUN   3LOAD"   4SAVE"   5CONT 6,"LPT1 7TRON 8TROFF9KEY    0SCREEN
```

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OF POOR QUALITY

```
O depleted by 100x; 5x solar C; 2x solar N
Temperature =  2000          Pressure =  4219.793 bars     50 iterations

                    Pressures of gases in bars
H = 9.848499E-02  H2 = 3686.705  He = 516.4525  Ne = .9715232
O = 2.604231E-12  O2 = 1.539627E-17  OH = 1.383737E-07  H2O = 5.015913E-02
N = 3.165769E-10  N2 = .1110481  NH3 = 1.526226  CN = 1.887765E-10
C = 8.672514E-14  CO = 2.997672E-04  CO2 = 9.005502E-10  CH4 = 13.78383
S = 1.191513E-07  S2 = 1.69864E-09  HS = 2.585057E-04  H2S = 9.329479E-02
C2H6 =  2.383315E-03  C2H4 =  1.026029E-03  C2H2 =  2.616713E-05
CH3OH =  4.551839E-07  HCHO =  1.145695E-06  HCOOH =  5.411673E-12
CH3NH2 =  4.769375E-05  CH3CN =  4.890698E-07  C2N2 =  1.231635E-12
N2H4 =  8.70589E-09  HCN =  7.728962E-04  CH3SH =  7.861448E-07  SO2 =
 2.854208E-16

INPUT ABUNDANCES OF ELEMENTS
H = 7433.529  O = 5.045995E-02  C = 13.79182  N = 1.748319  S = 9.355409E-02
                                     Graphite activity = 2.595007E-03
CALCULATED ABUNDANCES OF ELEMENTS
H = 7433.528  O = 5.045995E-02  C = 13.79182  N = 1.749143  S = .0935542
Type 1 to continue, 0 to end:
Ok


1LIST   2RUN   3LOAD"  4SAVE"  5CONT 6,"LPT1 7TRON 8TROFF9KEY    0SCREEN

O depleted by 100x; 5x solar C; 2x solar N
Temperature =  1800          Pressure =  2970.039 bars     50 iterations

                    Pressures of gases in bars
H = 1.816007E-02  H2 = 2594.873  He = 363.5012  Ne = .6837993
O = 7.376757E-14  O2 = 5.387644E-19  OH = 8.237055E-08  H2O = 3.546461E-02
N = 1.006833E-11  N2 = 7.584067E-02  NH3 = 1.079319  CN = 1.28533E-11
C = 3.013053E-16  CO = 5.10205E-05  CO2 = 1.847292E-10  CH4 = 9.706406
S = 1.503823E-08  S2 = 5.109267E-10  HS = 3.623548E-05  H2S = 6.580944E-02
C2H6 =  2.657121E-04  C2H4 =  6.373903E-05  C2H2 =  6.985194E-07
CH3OH =  6.997143E-08  HCHO =  1.38509E-07  HCOOH =  7.076101E-13
CH3NH2 =  8.324165E-06  CH3CN =  2.334907E-08  C2N2 =  1.811424E-14
N2H4 =  1.607567E-09  HCN =  1.425824E-04  CH3SH =  1.719891E-06  SO2 =
 6.08903E-17

INPUT ABUNDANCES OF ELEMENTS
H = 5232.033  O = 3.551585E-02  C = 9.707269  N = 1.230541  S = 6.584734E-02
                                     Graphite activity = 1.074172E-03
CALCULATED ABUNDANCES OF ELEMENTS
H = 5232.031  O = 3.551585E-02  C = 9.707269  N = 1.231151  S = 6.584741E-02
Type 1 to continue, 0 to end:
Ok


1LIST   2RUN   3LOAD"  4SAVE"  5CONT 6,"LPT1 7TRON 8TROFF9KEY    0SCREEN

O depleted by 100x; 5x solar C; 2x solar N
Temperature =  1500          Pressure =  1617.343 bars     70 iterations

                    Pressures of gases in bars
H = 6.593272E-04  H2 = 1413.002  He = 197.9564  Ne = .3723851
O = 1.040424E-16  O2 = 6.642071E-22  OH = 3.508905E-09  H2O = 1.933336E-02
N = 1.225023E-16  N2 = 4.076999E-06  NH3 = .6705073  CN = 2.780686E-16
C = 1.962038E-20  CO = 7.923487E-06  CO2 = 4.228545E-11  CH4 = 5.286119
S = 2.401176E-10  S2 = 4.559576E-11  HS = 2.792071E-06  H2S = .035856
C2H6 =  1.312869E-04  C2H4 =  8.876554E-06  C2H2 =  1.633878E-08
CH3OH =  1.092988E-08  HCHO =  1.221505E-08  HCOOH =  7.328848E-14
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CH3NH2 =  1.877937E-08  CH3CN =  1.974834E-11  C2N2 =  1.34901E-20
N2H4 =  7.614188E-15  HCN =  1.270661E-07  CH3SH =  5.40708E-07  SO2 =
 2.797316E-18

INPUT ABUNDANCES OF ELEMENTS
H = 2849.273  O = 1.934131E-02  C = 5.286409  N = .6701309  S = 3.585931E-02
                                    Graphite activity = 1.00669E-03
CALCULATED ABUNDANCES OF ELEMENTS
H = 2849.272  O = 1.934131E-02  C = 5.286408  N = .6705155  S = 3.585934E-02
Type 1 to continue, 0 to end:
Ok


1LIST   2RUN   3LOAD"   4SAVE"   5CONT 6,"LPT1 7TRON 8TROFF9KEY    0SCREEN

O depleted by 100x; 5x solar C; 2x solar N
Temperature =  1200          Pressure =  768.7372 bars      55 iterations

                  Pressures of gases in bars
H = 5.087248E-06  H2 = 671.6225  He = 94.08841  Ne = .1769942
O = 4.298771E-21  O2 = 2.9829E-26  OH = 3.450484E-11  H2O = 9.192716E-03
N = 3.791813E-19  N2 = 8.162363E-03  NH3 = .3023953  CN = 7.445251E-19
C = 3.924881E-27  CO = 1.833411E-07  CO2 = 1.839154E-12  CH4 = 2.512601
S = 4.880029E-13  S2 = 1.204775E-12  HS = 6.25235E-08  H2S = 1.704378E-02
C2H6 =  1.125174E-05  C2H4 =  9.636375E-08  C2H2 =  1.028781E-11
CH3OH =  3.730186E-10  HCHO =  1.486377E-10  HCOOH =  1.156163E-15
CH3NH2 =  8.428112E-08  CH3CN =  6.617255E-12  C2N2 =  6.555451E-22
N2H4 =  5.585369E-13  HCN =  1.012177E-07  CH3SH =  5.119796E-08  SO2 =
 2.871384E-20

INPUT ABUNDANCES OF ELEMENTS
H = 1354.256  O = .0091929  C = 2.512623  N = .3185124  S = 1.704388E-02
                                    Graphite activity = 3.523232E-04
CALCULATED ABUNDANCES OF ELEMENTS
H = 1354.255  O = .0091929  C = 2.512624  N = .3187202  S = .0170439
Type 1 to continue, 0 to end:
Ok


1LIST   2RUN   3LOAD"   4SAVE"   5CONT 6,"LPT1 7TRON 8TROFF9KEY    0SCREEN

O depleted by 100x; 5x solar C; 2x solar N
Temperature =  1000          Pressure =  418.6333 bars      60 iterations

                  Pressures of gases in bars
H = 4.320209E-08  H2 = 365.7439  He = 51.23862  Ne = .0963874
O = 1.851961E-25  O2 = 1.409335E-30  OH = 3.748373E-13  H2O = 5.006262E-03
N = 1.232957E-23  N2 = 1.729206E-03  NH3 = .1700969  CN = 1.701442E-23
C = 6.62001E-34  CO = 3.583243E-09  CO2 = 7.076463E-14  CH4 = 1.368321
S = 1.007761E-15  S2 = 3.212027E-14  HS = 1.527639E-09  H2S = 9.281752E-03
C2H6 =  1.047392E-06  C2H4 =  9.885394E-10  C2H2 =  5.370211E-16
CH3OH =  1.45447E-11  HCHO =  1.809351E-12  HCOOH =  1.870558E-17
CH3NH2 =  4.652938E-09  CH3CN =  2.024601E-14  C2N2 =  2.440019E-25
N2H4 =  5.690312E-15  HCN =  7.539063E-10  CH3SH =  5.440383E-09  SO2 =
 3.144657E-22

INPUT ABUNDANCES OF ELEMENTS
H = 737.5001  O = 5.006266E-03  C = 1.368323  N = .1734553  S = 9.28175E-03
                                    Graphite activity = 1.04913E-04
CALCULATED ABUNDANCES OF ELEMENTS
H = 737.5  O = 5.006266E-03  C = 1.368323  N = .1735553  S = 9.281759E-03
Type 1 to continue, 0 to end:
Ok
```

ORIGINAL PAGE IS
OF POOR QUALITY

```
1LIST   2RUN   3LOAD"   4SAVE"   5CONT 6,"LPT1 7TRON 8TROFF9KEY    0SCREEN
```

```
Use adiabat (1) or insert pressures (2)? 1
O depleted by 100x; 5x solar C; 2x solar N
Temperature =  800          Pressure =  198.9755 bars     60 iterations

                    Pressures of gases in bars
H = 3.811698E-11  H2 = 173.8364  He = 24.35378  Ne = 4.581306E-02
O = 5.577271E-32  O2 = 4.952734E-37  OH = 4.869619E-16  H2O = 2.379484E-03
N = 2.157185E-30  N2 = 1.431473E-04  NH3 = 8.223923E-02  CN = 1.501928E-30
C = 0  CO = 8.875572E-12  CO2 = 5.147592E-16  CH4 = .6503657
S = 9.896119E-20  S2 = 1.461816E-16  HS = 6.45086E-12  H2S = 4.411634E-03
C2H6 =  4.007302E-08  C2H4 =  1.458255E-12  C2H2 =  6.585225E-20
CH3OH =  1.894221E-13  HCHO =  3.121904E-15  HCOOH =  4.985739E-20
CH3NH2 =  9.973546E-11  CH3CN =  3.895991E-18  C2N2 =  3.656833E-32
N2H4 =  7.872921E-18  HCN =  4.493508E-13  CH3SH =  2.429193E-10  SO2 =
 4.001868E-25

INPUT ABUNDANCES OF ELEMENTS
H = 350.5348  O = 2.379484E-03  C = .6503658  N = 8.244355E-02  S =
 4.411628E-03
                                     Graphite activity = 1.537263E-05
CALCULATED ABUNDANCES OF ELEMENTS
H = 350.5346  O = 2.379484E-03  C = .6503658  N = 8.252553E-02  S =
 4.411634E-03
Type 1 to continue, 0 to end:
1LIST   2RUN  3LOAD"  4SAVE"  5CONT 6,"LPT1 7TRON 8TROFF9KEY    0SCREEN

O depleted by 100x; 5x solar C; 2x solar N
Temperature =  600          Pressure =  76.26708 bars     65 iterations

                    Pressures of gases in bars
H = 3.765497E-16  H2 = 66.63121  He = 9.334786  Ne = 1.756011E-02
O = 0  O2 = 0  OH = 9.555198E-21  H2O = 9.120544E-04
N = 0  N2 = 1.945015E-06  NH3 = .0316235  CN = 0
C = 0  CO = 3.714632E-16  CO2 = 0  CH4 = .2492847
S = 2.251161E-26  S2 = 2.696713E-17  HS = 8.494815E-16  H2S = 1.690976E-03
C2H6 =  3.237286E-10  C2H4 =  3.351467E-17  C2H2 =  4.243173E-18
CH3OH =  1.941765E-16  HCHO =  8.881815E-20  HCOOH =  0
CH3NH2 =  2.328658E-13  CH3CN =  2.517666E-24  C2N2 =  0
N2H4 =  1.923949E-22  HCN =  1.777272E-18  CH3SH =  1.976682E-12  SO2 =  0

INPUT ABUNDANCES OF ELEMENTS
H = 134.3597  O = 9.120544E-04  C = .2492847  N = 3.160055E-02  S =
 1.690973E-03
                                     Graphite activity = 5.60367E-07
CALCULATED ABUNDANCES OF ELEMENTS
H = 134.3596  O = 9.120544E-04  C = .2492847  N = 3.162739E-02  S =
 1.690976E-03
Type 1 to continue, 0 to end:
Ok

1LIST   2RUN  3LOAD"  4SAVE"  5CONT 6,"LPT1 7TRON 8TROFF9KEY    0SCREEN
```

```
Temperature = 2000
Use adiabat (1) or insert pressures (2)? 1

Water severely depleted; 4x solar C; 2x solar N
Temperature =  2000            Pressure =  4222.55 bars     50 iterations

                  Pressures of gases in bars
H = 9.855925E-02  H2 = 3692.267  He = 516.4525  Ne = .9715232
O = 2.184115E-15  O2 = 1.082947E-23  OH = 1.161387E-10  H2O = 4.21309E-05
N = 3.160501E-10  N2 = .1106789  NH3 = 1.527136  CN = 1.503344E-10
C = 6.91797E-14  CO = 2.005459E-07  CO2 = 5.052815E-16  CH4 = 11.02841
S = 1.189722E-07  S2 = 1.693537E-09  HS = 2.583118E-04  H2S = .0932951
C2H6 =  1.523396E-03  C2H4 =  6.548416E-04  C2H2 =  1.667547E-05
CH3OH =  3.0544E-10  HCHO =  7.676327E-10  HCOOH =  3.040968E-18
CH3NH2 =  3.81249E-05  CH3CN =  3.113846E-07  C2N2 =  7.810931E-13
N2H4 =  8.703143E-09  HCN =  6.159691E-04  CH3SH =  6.280474E-07  SO2 =
 2.004583E-22

INPUT ABUNDANCES OF ELEMENTS
H = 7433.529  O = 4.233217E-05  C = 11.03346  N = 1.748319  S = 9.355409E-02
                                   Graphite activity = 2.070009E-03
CALCULATED ABUNDANCES OF ELEMENTS
H = 7433.527  O = 4.233217E-05  C = 11.03346  N = 1.749148  S = 9.355416E-02
Type 1 to continue, 0 to end:
1LIST   2RUN   3LOAD"  4SAVE"  5CONT 6,"LPT1 7TRON 8TROFF9KEY    0SCREEN

Temperature = 1800
Use adiabat (1) or insert pressures (2)? 1

Water severely depleted; 4x solar C; 2x solar N
Temperature =  1800            Pressure =  2971.98 bars     50 iterations

                  Pressures of gases in bars
H = 1.817377E-02  H2 = 2598.79  He = 363.5012  Ne = .6837993
O = 6.18104E-17  O2 = 3.782605E-25  OH = 6.907098E-11  H2O = 2.976092E-05
N = 1.00508E-11  N2 = 7.557689E-02  NH3 = 1.079881  CN = 1.023402E-11
C = 2.403227E-16  CO = 3.4098E-08  CO2 = 1.034465E-16  CH4 = 7.765272
S = 1.501565E-08  S2 = 5.093931E-10  HS = 3.620836E-05  H2S = 6.580979E-02
C2H6 =  1.698058E-04  C2H4 =  4.067164E-05  C2H2 =  4.45051E-07
CH3OH =  4.690456E-11  HCHO =  9.270799E-11  HCOOH =  3.968527E-19
CH3NH2 =  6.652883E-06  CH3CN =  1.486181E-08  C2N2 =  1.148374E-14
N2H4 =  1.606815E-09  HCN =  1.136122E-04  CH3SH =  1.373873E-06  SO2 =
 4.268621E-23

INPUT ABUNDANCES OF ELEMENTS
H = 5232.033  O = 2.979518E-05  C = 7.765815  N = 1.230541  S = 6.584734E-02
                                   Graphite activity = 8.567654E-04
CALCULATED ABUNDANCES OF ELEMENTS
H = 5232.031  O = 2.979518E-05  C = 7.765816  N = 1.231155  S = 6.584738E-02
Type 1 to continue, 0 to end:
1LIST   2RUN   3LOAD"  4SAVE"  5CONT 6,"LPT1 7TRON 8TROFF9KEY    0SCREEN
```

```
Temperature = 1500
Use adiabat (1) or insert pressures (2)? 1

Water severely depleted; 4x solar C; 2x solar N
Temperature =  1500          Pressure =  1618.401 bars     70 iterations

                    Pressures of gases in bars
H = 6.598249E-04  H2 = 1415.136  He = 197.9564  Ne = .3723851
O = 8.715959E-20  O2 = 4.661363E-28  OH = 2.941738E-12  H2O = 1.622062E-05
N = 1.222253E-16  N2 = 4.05858E-06  NH3 = .670507  CN = 2.212856E-16
C = 1.564919E-20  CO = 5.294263E-09  CO2 = 2.366926E-17  CH4 = 4.228946
S = 2.397563E-10  S2 = 4.545866E-11  HS = 2.789974E-06  H2S = 3.585612E-02
C2H6 =  8.389894E-05  C2H4 =  5.66401E-06  C2H2 =  1.040984E-08
CH3OH =  7.325129E-12  HCHO =  8.174095E-12  HCOOH =  4.108515E-20
CH3NH2 =  1.500101E-08  CH3CN =  1.256317E-11  C2N2 =  8.543137E-21
N2H4 =  7.6027E-15  HCN =  1.011949E-07  CH3SH =  4.319208E-07  SO2 =
 1.960185E-24

INPUT ABUNDANCES OF ELEMENTS
H = 2849.273  O = 1.622593E-05  C = 4.229126  N = .6701309  S = 3.585931E-02
                                 Graphite activity = 8.029344E-04
CALCULATED ABUNDANCES OF ELEMENTS
H = 2849.272  O = 1.622593E-05  C = 4.229126  N = .6705152  S = 3.585934E-02
Type 1 to continue, 0 to end:
1LIST   2RUN  3LOAD"  4SAVE"  5CONT 6,"LPT1 7TRON 8TROFF9KEY    0SCREEN

Temperature = 1200
Use adiabat (1) or insert pressures (2)? 1

Water severely depleted; 4x solar C; 2x solar N
Temperature =  1200          Pressure =  769.2399 bars     55 iterations

                    Pressures of gases in bars
H = 5.091088E-06  H2 = 672.6368  He = 94.08841  Ne = .1769942
O = 3.600928E-24  O2 = 2.093047E-32  OH = 2.89253E-14  H2O = 7.712042E-06
N = 3.784081E-19  N2 = 8.129111E-03  NH3 = .3024626  CN = 5.926152E-19
C = 3.130446E-27  CO = 1.224926E-10  CO2 = 1.029291E-18  CH4 = 2.010084
S = 4.872674E-13  S2 = 1.201146E-12  HS = 6.247638E-08  H2S = 1.704379E-02
C2H6 =  7.190275E-06  C2H4 =  6.148713E-08  C2H2 =  6.554474E-12
CH3OH =  2.499719E-13  HCHO =  9.945679E-14  HCOOH =  6.480291E-22
CH3NH2 =  6.733833E-08  CH3CN =  4.210506E-12  C2N2 =  4.153263E-22
N2H4 =  5.579431E-13  HCN =  8.062643E-08  CH3SH =  4.08967E-08  SO2 =
 2.011761E-26

INPUT ABUNDANCES OF ELEMENTS
H = 1354.256  O = 7.712164E-06  C = 2.010099  N = .3185124  S = 1.704388E-02
                                 Graphite activity = 2.810095E-04
CALCULATED ABUNDANCES OF ELEMENTS
H = 1354.255  O = 7.712165E-06  C = 2.010098  N = .318721  S = .0170439
Type 1 to continue, 0 to end:
1LIST   2RUN  3LOAD"  4SAVE"  5CONT 6,"LPT1 7TRON 8TROFF9KEY    0SCREEN
```

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```
Temperature = 1000
Use adiabat (1) or insert pressures (2)? 1

Water severely depleted; 4x solar C; 2x solar N
Temperature =  1000          Pressure =  418.907 bars     60 iterations

                  Pressures of gases in bars
H = 4.32347E-08  H2 = 366.2962  He = 51.23862  Ne = .0963874
O = 1.551316E-28  O2 = 9.888972E-37  OH = 3.142237E-16  H2O = 4.199884E-06
N = 1.23028E-23  N2 = 1.721704E-03  NH3 = .1701121  CN = 1.354106E-23
C = 5.280051E-34  CO = 2.394E-12  CO2 = 3.96034E-20  CH4 = 1.094657
S = 1.006242E-15  S2 = 3.202348E-14  HS = 1.526487E-09  H2S = 9.281751E-03
C2H6 =  6.693206E-07  C2H4 =  6.307591E-10  C2H2 =  3.421414E-16
CH3OH =  9.746829E-15  HCHO =  1.210671E-15  HCOOH =  1.048438E-23
CH3NH2 =  3.717071E-09  CH3CN =  1.288063E-14  C2N2 =  1.545482E-25
N2H4 =  5.682748E-15  HCN =  6.004549E-10  CH3SH =  4.345745E-09  SO2 =
 2.203204E-28

INPUT ABUNDANCES OF ELEMENTS
H = 737.5001  O = 4.199887E-06  C = 1.094659  N = .1734553  S = 9.28175E-03
                                  Graphite activity = 8.36775E-05
CALCULATED ABUNDANCES OF ELEMENTS
H = 737.4999  O = 4.199887E-06  C = 1.094659  N = .1735555  S = 9.281758E-03
Type 1 to continue, 0 to end:
1LIST   2RUN   3LOAD"   4SAVE"   5CONT 6,"LPT1 7TRON 8TROFF9KEY    0SCREEN

Temperature = 800
Use adiabat (1) or insert pressures (2)? 1

Water severely depleted; 4x solar C; 2x solar N
Temperature =  800           Pressure =  199.1056 bars     60 iterations

                  Pressures of gases in bars
H = 3.814574E-11  H2 = 174.0989  He = 24.35378  Ne = 4.581306E-02
O = 4.671863E-35  O2 = 0  OH = 4.082169E-19  H2O = 1.996211E-06
N = 2.152343E-30  N2 = 1.425054E-04  NH3 = 8.224059E-02  CN = 1.195233E-30
C = 0  CO = 5.929854E-15  CO2 = 0  CH4 = .5202926
S = 9.881199E-20  S2 = 1.457411E-16  HS = 6.445996E-12  H2S = 4.411634E-03
C2H6 =  2.560806E-08  C2H4 =  9.304709E-13  C2H2 =  4.195508E-20
CH3OH =  1.269372E-16  HCHO =  2.088923E-18  HCOOH =  0
CH3NH2 =  7.966937E-11  CH3CN =  2.47847E-18  C2N2 =  2.315859E-32
N2H4 =  7.86131E-18  HCN =  3.578628E-13  CH3SH =  1.940424E-10  SO2 =  0

INPUT ABUNDANCES OF ELEMENTS
H = 350.5348  O = 1.996212E-06  C = .5202926  N = 8.244354E-02  S =
 4.411628E-03
                                  Graphite activity = 1.226104E-05
CALCULATED ABUNDANCES OF ELEMENTS
H = 350.5346  O = 1.996211E-06  C = .5202926  N = .0825256  S = 4.411634E-03
Type 1 to continue, 0 to end:
1LIST   2RUN   3LOAD"   4SAVE"   5CONT 6,"LPT1 7TRON 8TROFF9KEY    0SCREEN
```

```
Use adiabat (1) or insert pressures (2)? 1

Water severely depleted; 4x solar C; 2x solar N
Temperature =  600            Pressure =  76.31692 bars      65 iterations

                    Pressures of gases in bars
H = 3.768339E-16  H2 = 66.73183  He = 9.334786  Ne = 1.756011E-02
O = 0  O2 = 0  OH = 8.010059E-24  H2O = 7.651463E-07
N = 0  N2 = 1.936232E-06  NH3 = 3.162351E-02  CN = 0
C = 0  CO = 2.481781E-19  CO2 = 0  CH4 = .1994278
S = 2.247766E-26  S2 = 2.688586E-17  HS = 8.488406E-16  H2S = 1.690976E-03
C2H6 =  2.068738E-10  C2H4 =  2.138475E-17  C2H2 =  2.703365E-18
CH3OH =  1.301233E-19  HCHO =  5.942987E-23  HCOOH =  0
CH3NH2 =  1.860118E-13  CH3CN =  1.60161E-24  C2N2 =  0
N2H4 =  1.921049E-22  HCN =  1.415396E-18  CH3SH =  1.578961E-12  SO2 =  0

INPUT ABUNDANCES OF ELEMENTS
H = 134.3597  O = 7.651463E-07  C = .1994277  N = 3.160054E-02  S =
 1.690973E-03
                                      Graphite activity = 4.469427E-07
CALCULATED ABUNDANCES OF ELEMENTS
H = 134.3596  O = 7.651463E-07  C = .1994278  N = 3.162738E-02  S =
 1.690976E-03
Type 1 to continue, 0 to end:
1LIST   2RUN   3LOAD"  4SAVE"  5CONT 6,"LPT1 7TRON 8TROFF9KEY    0SCREEN
```

```
O depleted by 10x; 5x solar C; 2x solar N:  Lightning discharge
Temperature =  2000          Pressure =  49.87719 bars      18 iterations

                  Pressures of gases in bars
H = 1.070872E-02  H2 = 43.58863  He = 6.100001  Ne = .011475
O = 6.501539E-13  O2 = 9.595968E-19  OH = 3.756277E-09  H2O = 1.480545E-04
N = 9.068982E-11  N2 = 9.113181E-03  NH3 = 5.62083E-04  CN = 4.199784E-09
C = 6.73511E-12  CO = 5.811931E-03  CO2 = 4.35894E-09  CH4 = .1496371
S = 1.163633E-07  S2 = 1.620078E-09  HS = 2.74508E-05  H2S = 1.077233E-03
C2H6 =  2.375666E-05  C2H4 =  8.650247E-04  C2H2 =  1.865909E-03
CH3OH =  1.233653E-09  HCHO =  2.626276E-07  HCOOH =  3.096987E-13
CH3NH2 =  1.61279E-08  CH3CN =  1.086305E-06  C2N2 =  6.095932E-10
N2H4 =  9.987153E-14  HCN =  1.869681E-03  CH3SH =  8.334689E-09  SO2 =
 1.737306E-17

INPUT ABUNDANCES OF ELEMENTS
H = 87.8  O = .00596  C = .1629  N = .02065  S = .001105
                                   Graphite activity = .2015293
CALCULATED ABUNDANCES OF ELEMENTS
H = 87.79988  O = 5.960001E-03  C = .1628306  N = 2.065923E-02  S =
 1.104812E-03
Type 1 to continue, 0 to end:
Ok

1LIST   2RUN   3LOAD"   4SAVE"   5CONT 6,"LPT1 7TRON 8TROFF9KEY    0SCREEN

O depleted by 10x; 5x solar C; 2x solar N:  Lightning discharge
Temperature =  1800          Pressure =  44.88272 bars      18 iterations

                  Pressures of gases in bars
H = 2.232697E-03  H2 = 39.22298  He = 5.49  Ne = .0103275
O = 1.044425E-13  O2 = 1.079997E-18  OH = 1.433825E-08  H2O = 7.589819E-04
N = 3.422217E-12  N2 = 8.761989E-03  NH3 = 6.817684E-04  CN = 2.785055E-10
C = 1.920771E-14  CO = 4.604954E-03  CO2 = 2.36063E-08  CH4 = .1413762
S = 1.496627E-08  S2 = 5.060485E-10  HS = 4.433667E-06  H2S = 9.899868E-04
C2H6 =  3.729257E-06  C2H4 =  5.918232E-05  C2H2 =  4.290822E-05
CH3OH =  1.442947E-09  HCHO =  1.889657E-07  HCOOH =  1.366819E-12
CH3NH2 =  5.066652E-09  CH3CN =  5.993686E-08  C2N2 =  8.504686E-12
N2H4 =  4.243445E-14  HCN =  3.79837E-04  CH3SH =  2.493076E-08  SO2 =
 1.214754E-16

INPUT ABUNDANCES OF ELEMENTS
H = 79.02001  O = 5.364001E-03  C = .14661  N = .018585  S = .0009945
                                   Graphite activity = 6.847667E-02
CALCULATED ABUNDANCES OF ELEMENTS
H = 79.01996  O = .005364  C = .146573  N = 1.858565E-02  S = 9.944614E-04
Type 1 to continue, 0 to end:
Ok

1LIST   2RUN   3LOAD"   4SAVE"   5CONT 6,"LPT1 7TRON 8TROFF9KEY    0SCREEN
```

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O depleted by 10x; 5x solar C; 2x solar N:  Lightning discharge
Temperature =  1500          Pressure =  37.38291 bars      60 iterations

                    Pressures of gases in bars
H = 1.002367E-04  H2 = 32.65836  He = 4.575  Ne = 8.606251E-03
O = 5.930467E-16  O2 = 2.158044E-20  OH = 3.040716E-09  H2O = 2.547049E-03
N = 7.879071E-16  N2 = 1.686561E-04  NH3 = 1.515345E-02  CN = 7.614259E-14
C = 8.353191E-19  CO = 1.922825E-03  CO2 = 5.849149E-08  CH4 = .1202223
S = 2.399968E-10  S2 = 4.554991E-11  HS = 4.242616E-07  H2S = 8.283139E-04
C2H6 =  2.938098E-06  C2H4 =  8.594836E-06  C2H2 =  6.844807E-07
CH3OH =  1.416909E-09  HCHO =  6.851255E-08  HCOOH =  2.34309E-12
CH3NH2 =  4.176242E-10  CH3CN =  8.08963E-10  C2N2 =  1.011501E-15
N2H4 =  1.682628E-16  HCN =  5.2897E-06  CH3SH =  1.229115E-08  SO2 =
 9.084054E-17

INPUT ABUNDANCES OF ELEMENTS
H = 65.85001  O = .00447  C = .122175  N = .0154875  S = 8.2875E-04
                                     Graphite activity = 4.285886E-02
CALCULATED ABUNDANCES OF ELEMENTS
H = 65.84999  O = 4.469997E-03  C = .122175  N = 1.549606E-02  S = 8.287508E-04

Type 1 to continue, 0 to end:
Ok

1LIST   2RUN   3LOAD"   4SAVE"   5CONT 6,"LPT1 7TRON 8TROFF9KEY    0SCREEN

O depleted by 10x; 5x solar C; 2x solar N:  Lightning discharge
Temperature =  1200          Pressure =  29.91357 bars      15 iterations

                    Pressures of gases in bars
H = 1.003583E-06  H2 = 26.13762  He = 3.66  Ne = .006885
O = 4.241115E-20  O2 = 2.903423E-24  OH = 6.715621E-11  H2O = 3.529558E-03
N = 3.045723E-19  N2 = 5.266269E-03  NH3 = 1.864789E-03  CN = 1.535244E-17
C = 1.007583E-25  CO = 4.643548E-05  CO2 = 4.595619E-09  CH4 = 9.769209E-02
S = 4.877596E-13  S2 = 1.203574E-12  HS = 1.232812E-08  H2S = 6.629643E-04
C2H6 =  4.370697E-07  C2H4 =  9.618427E-08  C2H2 =  2.638593E-10
CH3OH =  1.430877E-10  HCHO =  1.465076E-09  HCOOH =  1.124309E-13
CH3NH2 =  5.192546E-10  CH3CN =  2.689314E-11  C2N2 =  2.787396E-19
N2H4 =  5.457837E-16  HCN =  4.117416E-07  CH3SH =  1.989629E-09  SO2 =
 2.793484E-18

INPUT ABUNDANCES OF ELEMENTS
H = 52.68  O = .003576  C = 9.774001E-02  N = .01239  S = 6.630001E-04
                                     Graphite activity = 9.044731E-03
CALCULATED ABUNDANCES OF ELEMENTS
H = 52.67999  O = 3.576003E-03  C = 9.774001E-02  N = 1.239774E-02  S =
 6.629786E-04
Type 1 to continue, 0 to end:
Ok

1LIST   2RUN   3LOAD"   4SAVE"   5CONT 6,"LPT1 7TRON 8TROFF9KEY    0SCREEN
```

Appendix 7 50 A7

```
O depleted by 100x; 5x solar C; 2x solar N:  Lightning discharge
Temperature =  2000          Pressure =  49.86685 bars      18 iterations

                    Pressures of gases in bars
H = 1.070751E-02  H2 = 43.57882  He = 6.100001  Ne = .011475
O = 6.299005E-14  O2 = 9.007418E-21  OH = 3.638853E-10  H2O = 1.4341E-05
N = 9.054086E-11  N2 = 9.083266E-03  NH3 = 5.609702E-04  CN = 4.331166E-09
C = 6.957232E-12  CO = 5.816583E-04  CO2 = 4.226533E-11  CH4 = .1545025
S = 1.164111E-07  S2 = 1.62141E-09  HS = 2.745899E-05  H2S = 1.077433E-03
C2H6 =  2.533236E-05  C2H4 =  9.226067E-04  C2H2 =  1.990564E-03
CH3OH =  1.234085E-10  HCHO =  2.627787E-08  HCOOH =  3.002237E-15
CH3NH2 =  1.662307E-08  CH3CN =  1.156844E-06  C2N2 =  6.483294E-10
N2H4 =  9.949889E-14  HCN =  1.927954E-03  CH3SH =  8.609225E-09  SO2 =
 1.631422E-19

INPUT ABUNDANCES OF ELEMENTS
H = 87.8  O = .000596  C = .1629  N = .02065  S = .001105
                                      Graphite activity = .2081757
CALCULATED ABUNDANCES OF ELEMENTS
H = 87.80001  O = .000596  C = .1628915  N = 2.065663E-02  S = 1.10502E-03
Type 1 to continue, 0 to end:
Ok


1LIST   2RUN   3LOAD"   4SAVE"   5CONT 6,"LPT1 7TRON 8TROFF9KEY    0SCREEN

O depleted by 10x; 5x solar C; 2x solar N:  Lightning discharge
Temperature =  1800          Pressure =  44.8745 bars      15 iterations

                    Pressures of gases in bars
H = 2.232483E-03  H2 = 39.21545  He = 5.49  Ne = .0103275
O = 1.018887E-14  O2 = 1.027826E-20  OH = 1.39863E-09  H2O = 7.40281E-05
N = 3.421168E-12  N2 = 8.75662E-03  NH3 = 6.813632E-04  CN = 2.86714E-10
C = 1.977989E-14  CO = 4.626175E-04  CO2 = 2.313521E-10  CH4 = .1455318
S = 1.496648E-08  S2 = 5.060624E-10  HS = 4.433303E-06  H2S = 9.898106E-04
C2H6 =  3.952471E-06  C2H4 =  6.273671E-05  C2H2 =  4.549396E-05
CH3OH =  1.44904E-10  HCHO =  1.898001E-08  HCOOH =  1.339285E-14
CH3NH2 =  5.21348E-09  CH3CN =  6.352321E-08  C2N2 =  9.0134E-12
N2H4 =  4.239216E-14  HCN =  3.909945E-04  CH3SH =  2.566392E-08  SO2 =
 1.15609E-18

INPUT ABUNDANCES OF ELEMENTS
H = 79.02001  O = .0005364  C = .14661  N = .018585  S = .0009945
                                      Graphite activity = 7.051653E-02
CALCULATED ABUNDANCES OF ELEMENTS
H = 79.02018  O = 5.366478E-04  C = .1466099  N = 1.858567E-02  S =
 9.942854E-04
Type 1 to continue, 0 to end:
Ok

1LIST   2RUN   3LOAD"   4SAVE"   5CONT 6,"LPT1 7TRON 8TROFF9KEY    0SCREEN
```

O depleted by 10x; 5x solar C; 2x solar N: Lightning discharge
Temperature = 2000 Pressure = 9.980935 bars 33 iterations

Pressures of gases in bars
H = 4.792545E-03 H2 = 8.730329 He = 1.22 Ne = .002295
O = 3.878059E-14 O2 = 3.414171E-21 OH = 1.002731E-10 H2O = 1.768794E-06
N = 3.650441E-11 N2 = 1.476534E-03 NH3 = 2.028025E-05 CN = 5.803986E-09
C = 2.31237E-11 CO = 1.190231E-03 CO2 = 5.324636E-11 CH4 = 2.060946E-02
S = 1.127089E-07 S2 = 1.519918E-09 HS = 1.189942E-05 H2S = 2.089821E-04
C2H6 = 2.250001E-06 C2H4 = 4.090426E-04 C2H2 = 4.405274E-03
CH3OH = 1.013488E-11 HCHO = 1.07723E-08 HCOOH = 7.577149E-16
CH3NH2 = 4.00148E-10 CH3CN = 4.620084E-07 C2N2 = 1.16423E-09
N2H4 = 6.491276E-16 HCN = 1.156367E-03 CH3SH = 1.111882E-09 SO2 =
5.987076E-20

INPUT ABUNDANCES OF ELEMENTS
H = 17.56 O = .001192 C = .03258 N = .00413 S = .000221
Graphite activity = .691912
CALCULATED ABUNDANCES OF ELEMENTS
H = 17.56 O = .001192 C = 3.259014E-02 N = 4.130187E-03 S = 2.209984E-04
Type 1 to continue, 0 to end:
Ok

1LIST 2RUN 3LOAD" 4SAVE" 5CONT 6,"LPT1 7TRON 8TROFF9KEY 0SCREEN

O depleted by 10x; 5x solar C; 2x solar N: Lightning discharge
Temperature = 1800 Pressure = 9.974824 bars 23 iterations

Pressures of gases in bars
H = 1.052588E-03 H2 = 8.717609 He = 1.22 Ne = .002295
O = 6.128183E-15 O2 = 3.718188E-21 OH = 3.966239E-10 H2O = 9.897892E-06
N = 1.580012E-12 N2 = 1.867705E-03 NH3 = 3.298184E-05 CN = 5.625504E-10
C = 8.403311E-14 CO = 1.182101E-03 CO2 = 3.555591E-10 CH4 = 3.055377E-02
S = 1.488891E-08 S2 = 5.008308E-10 HS = 2.079414E-06 H2S = 2.18895E-04
C2H6 = 7.836869E-07 C2H4 = 5.595713E-05 C2H2 = 1.825354E-04
CH3OH = 1.829757E-11 HCHO = 1.078125E-08 HCOOH = 4.575636E-15
CH3NH2 = 2.383366E-10 CH3CN = 5.549858E-08 C2N2 = 3.469873E-11
N2H4 = 4.468252E-16 HCN = 3.61704E-04 CH3SH = 5.360108E-09 SO2 =
4.160512E-19

INPUT ABUNDANCES OF ELEMENTS
H = 17.56 O = .001192 C = .03258 N = .00413 S = .000221
Graphite activity = .2995833
CALCULATED ABUNDANCES OF ELEMENTS
H = 17.56 O = .001192 C = 3.257625E-02 N = 4.130151E-03 S = 2.209956E-04
Type 1 to continue, 0 to end:
Ok

1LIST 2RUN 3LOAD" 4SAVE" 5CONT 6,"LPT1 7TRON 8TROFF9KEY 0SCREEN

```
O depleted by 10x; 5x solar C; 2x solar N:  Lightning discharge
Temperature =  1500          Pressure =  9.970698 bars     45 iterations

                  Pressures of gases in bars
H = 5.17706E-05  H2 = 8.711785  He = 1.22  Ne = .002295
O = 9.122366E-17  O2 = 5.106196E-22  OH = 2.415744E-10  H2O = 1.045126E-04
N = 1.238705E-15  N2 = 4.168575E-04  NH3 = 3.282264E-03  CN = 4.401309E-13
C = 3.07124E-18  CO = 1.087476E-03  CO2 = 5.088518E-09  CH4 = 3.145372E-02
S = 2.398021E-10  S2 = 4.547602E-11  HS = 2.189462E-07  H2S = 2.207777E-04
C2H6 =  7.539234E-07  C2H4 =  8.267721E-06  C2H2 =  2.468293E-06
CH3OH =  5.702265E-11  HCHO =  1.033625E-08  HCOOH =  5.437514E-14
CH3NH2 =  8.872005E-11  CH3CN =  2.368718E-09  C2N2 =  3.379673E-14
N2H4 =  2.95937E-17  HCN =  1.579216E-05  CH3SH =  3.213119E-09  SO2 =
 2.147655E-18

INPUT ABUNDANCES OF ELEMENTS
H = 17.56  O = .001192  C = .03258  N = .00413  S = .000221
                                   Graphite activity = .1575803
CALCULATED ABUNDANCES OF ELEMENTS
H = 17.56  O = 1.191999E-03  C = 3.257999E-02  N = 4.131774E-03  S =
 2.210002E-04
Type 1 to continue, 0 to end:
Ok

1LIST   2RUN   3LOAD"   4SAVE"   5CONT 6,"LPT1 7TRON 8TROFF9KEY    0SCREEN

O depleted by 10x; 5x solar C; 2x solar N:  Lightning discharge
Temperature =  1200          Pressure =  9.971814 bars     15 iterations

                  Pressures of gases in bars
H = 5.794502E-07  H2 = 8.713478  He = 1.22  Ne = .002295
O = 3.843064E-20  O2 = 2.383996E-24  OH = 3.513553E-11  H2O = 1.066212E-03
N = 1.855947E-19  N2 = 1.95548E-03  NH3 = 2.187224E-04  CN = 2.79641E-17
C = 3.011821E-25  CO = 1.257754E-04  CO2 = 1.127944E-08  CH4 = 3.245331E-02
S = 4.876982E-13  S2 = 1.203271E-12  HS = 7.117135E-09  H2S = 2.209841E-04
C2H6 =  1.446852E-07  C2H4 =  9.551067E-08  C2H2 =  7.859496E-10
CH3OH =  4.307241E-11  HCHO =  1.322914E-09  HCOOH =  9.199301E-14
CH3NH2 =  6.069008E-11  CH3CN =  2.818394E-11  C2N2 =  9.247952E-19
N2H4 =  2.252278E-17  HCN =  4.330231E-07  CH3SH =  6.608712E-10  SO2 =
 2.293437E-18

INPUT ABUNDANCES OF ELEMENTS
H = 17.56  O = .001192  C = .03258  N = .00413  S = .000221
                                   Graphite activity = .0270361
CALCULATED ABUNDANCES OF ELEMENTS
H = 17.56  O = 1.19201E-03  C = 3.258001E-02  N = 4.130115E-03  S =
 2.209919E-04
Type 1 to continue, 0 to end:
Ok

1LIST   2RUN   3LOAD"   4SAVE"   5CONT 6,"LPT1 7TRON 8TROFF9KEY    0SCREEN
```

```
O depleted by 100x; 5x solar C; 2x solar N:  Lightning discharge
Temperature =  2000           Pressure =  9.979018 bars      33 iterations

                   Pressures of gases in bars
H = 4.792168E-03  H2 = 8.728957  He = 1.22  Ne = .002295
O = 3.777804E-15  O2 = 3.239926E-23  OH = 9.767319E-12  H2O = 1.722796E-07
N = 3.63475E-11  N2 = 1.463868E-03  NH3 = 2.018832E-05  CN = 5.932633E-09
C = 2.373828E-11  CO = 1.190277E-04  CO2 = 5.187185E-13  CH4 = 2.115057E-02
S = 1.127254E-07  S2 = 1.520363E-09  HS = 1.190022E-05  H2S = 2.089798E-04
C2H6 =  2.370073E-06  C2H4 =  4.30939E-04  C2H2 =  4.641822E-03
CH3OH =  1.013209E-12  HCHO =  1.077103E-09  HCOOH =  7.380391E-18
CH3NH2 =  4.088567E-10  CH3CN =  4.846861E-07  C2N2 =  1.216413E-09
N2H4 =  6.433568E-16  HCN =  1.181905E-03  CH3SH =  1.141242E-09  SO2 =
 5.682353E-22

INPUT ABUNDANCES OF ELEMENTS
H = 17.56  O = .0001192  C = .03258  N = .00413  S = .000221
                                   Graphite activity = .7103015
CALCULATED ABUNDANCES OF ELEMENTS
H = 17.56  O = .0001192  C = 3.260275E-02  N = 4.130323E-03  S = 2.20997E-04
Type 1 to continue, 0 to end:
Ok


1LIST   2RUN   3LOAD"   4SAVE"   5CONT 6,"LPT1 7TRON 8TROFF9KEY    0SCREEN

O depleted by 100x; 5x solar C; 2x solar N:  Lightning discharge
Temperature =  1800           Pressure =  9.972706 bars      18 iterations

                   Pressures of gases in bars
H = 1.052463E-03  H2 = 8.715545  He = 1.22  Ne = .002295
O = 5.928473E-16  O2 = 3.479794E-23  OH = 3.836529E-11  H2O = 9.573064E-07
N = 1.577683E-12  N2 = 1.862203E-03  NH3 = 3.292153E-05  CN = 5.808037E-10
C = 8.688782E-14  CO = 1.182427E-04  CO2 = 3.440665E-12  CH4 = 3.157677E-02
S = 1.489276E-08  S2 = 5.010895E-10  HS = 2.079705E-06  H2S = 2.188996E-04
C2H6 =  8.372421E-07  C2H4 =  5.979526E-05  C2H2 =  1.951018E-04
CH3OH =  1.829394E-12  HCHO =  1.078167E-09  HCOOH =  4.426693E-17
CH3NH2 =  2.459244E-10  CH3CN =  5.922487E-08  C2N2 =  3.698703E-11
N2H4 =  4.45298E-16  HCN =  3.733961E-04  CH3SH =  5.541004E-09  SO2 =
 3.894765E-21

INPUT ABUNDANCES OF ELEMENTS
H = 17.56  O = .0001192  C = .03258  N = .00413  S = .000221
                                   Graphite activity = .3097605
CALCULATED ABUNDANCES OF ELEMENTS
H = 17.56  O = .0001192  C = .03258  N = 4.130784E-03  S = 2.210008E-04
Type 1 to continue, 0 to end:
Ok


1LIST   2RUN   3LOAD"   4SAVE"   5CONT 6,"LPT1 7TRON 8TROFF9KEY    0SCREEN
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II

Venus: Halide Cloud Condensation and Volatile Element Inventories

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Venus: Halide Cloud Condensation and Volatile Element Inventories

Abstract. *Several recently suggested Venus cloud condensates, including aluminum chloride and 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 be sufficiently volatile, but the expected molecular form is gaseous antimony sulfide, 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 arsenic and antimony. Thus arguments for a volatile-deficient origin for Venus based on depletion of water and mercury (relative to the earth) cannot be tested by a search for atmospheric arsenic or antimony.*

Soviet spacecraft have analyzed cloud particles in the main Venus cloud layer by means of x-ray fluorescence (XRF) spectroscopy (*1*). On the basis of these analyses it is claimed that chlorine is present as a cloud constituent and sulfur is not detected. These 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*). Direct evidence regarding the abundances of these species in the lower troposphere is lacking: copious production of COS and so on 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*). No composition data are available for the bottom 22 km of the atmosphere, a region which contains not only the best-equilibrated gases, but also over 80 percent of the total atmospheric mass.

The source of a chlorine-bearing aerosol is less obvious. We have 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, mercury, 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 the earth. Combined condensation-accretion models with a variety of recent estimates of the accretion sampling functions of the terrestrial planets (*7*) show a primordial water content on Venus from 10^{-1} to as low as 10^{-4} of the terrestrial value. The failure of the 1978 Pioneer Venus mission to detect even a trace of mercury in the lower atmosphere (*5*) strongly implies that Venus is deficient in mercury relative to the earth. The severe depletion of the most abundant terrestrial volatile, H_2O, on Venus is well known and is attributed to either a lack of water in preplanetary solids at the orbit of Venus (*8*) or massive loss of oceans of H_2 after differentiation and outgassing of the planet (*9*). Donahue (*10*) found an enhancement of the D/H ratio on Venus by about a factor of 100 over the terrestrial value, requiring either loss of hydrogen from 100 times the present water inventory or accumulation of deuterium-rich material on Venus. Such a late loss mechanism could not deplete mercury while leaving vast amounts of the lighter and more volatile species N_2 and CO_2. Thus the observed severe depletion of mercury 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 (*11*) suggested Al_2Cl_6 as the major cloud layer constituent and Barsukov *et al.* (*12*) suggested arsenic and antimony halides and oxides. Mole fractions of at least 10 ppm of condensable gases are required to provide the observed cloud density (*13*). Are these species plausible cloud constituents? Can useful limits on the abundances of the volatile elements arsenic and antimony be derived from atmospheric measurements?

It is simple to estimate the volatility of aluminum compounds at the mean surface conditions of Venus. Consider coexisting anorthite ($CaAl_2Si_2O_8$), quartz (SiO_2), and calcite ($CaCO_3$) at 750 K and 95 bars in contact with the atmosphere

$$CaAl_2Si_2O_8 + CO_2(g) + 6HCl(g) = CaCO_3 + 2SiO_2 + 3H_2O(g) + 2AlCl_3 \quad (1)$$

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The equilibrium constant for this reaction at this temperature is $10^{-26.1}$. Assuming the spectroscopic HCl abundance in the clouds, about 1 ppm (*14*), and the most typical water vapor abundance figures for the lower atmosphere, about 100 ppm (*15*), an $AlCl_3$ partial pressure of $10^{-21.0}$ bar is calculated. With an extreme effort to bias the equilibrium in favor of $AlCl_3$ production (raising HCl to 10 ppm and lowering H_2O to 10 ppm), we can force the $AlCl_3$ pressure only as high as $10^{-16.5}$ bar. This is still ten 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 (*16, 17*) and from surface passive gamma-ray spectroscopy (*18*). The surface of Venus lies, as accurately as can be determined, precisely on the calcite-quartz-wollastonite ($CaSiO_3$) buffer

$$CaCO_3 + SiO_2 = CaSiO_3 + CO_2(g) \quad (2)$$

and calcite is therefore also a plausible surface mineral. Since weathering reactions at higher altitudes on Venus will preferentially tend to mobilize a fine calcium-rich dust, which can be transported readily by winds to the hot lowlands, this buffer may not be difficult to establish on Venus (*19*).

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 (*20, 21*). We will calculate the partial pressures of a number of arsenic and antimony gases at the surface as a function of the activities of arsenic and antimony: an activity of 1 means the pure element is present on the surface and 10^{-4} means 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. Figure 1 presents the results for arsenic (*22*). For activities greater than about 10^{-2} the dominant gas is As_4, with As_4O_6 second. Based on 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 arsenic activities. This, in turn, places firm upper limits on the pressures of arsenic-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 antimony activities, SbS is the dominant gas. The best available data on Sb_2S_3 (stibnite) from Johnson *et al.* (*20*) 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 antimony 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} bar are conceivable for SbS and cannot be ruled out.

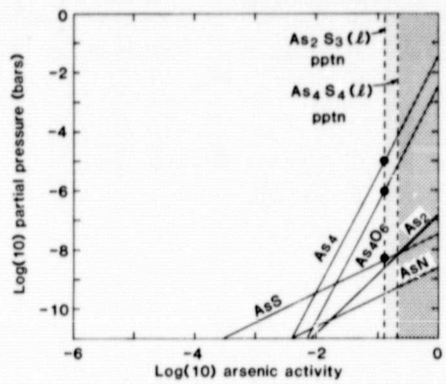

Fig. 1. Partial pressures of arsenic gases as a function of elemental arsenic activity at the Venus surface. Limitations of the arsenic activity imposed by precipitation of liquids of As_2S_3 (orpiment) and As_4S_4 (realgar) composition are indicated by vertical dashed lines. Heavy dots indicate the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

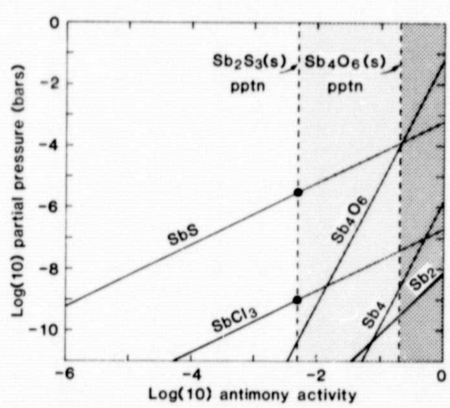

Fig. 2. Partial pressure of antimony gases as a function of elemental antimony activity. The Sb_4O_6 (valentinite) and Sb_2S_3 (stibnite) precipitation points are indicated by vertical dashed lines. Firm upper limits on the antimony gas pressures are indicated by the dots. The maximum total mole fraction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

Observational constraints on the abundance of arsenic in the Venus atmosphere even down to the level of 0.1 ppm are therefore not sufficient to test whether arsenic is, like water and mercury, depleted in Venus relative to the earth: the stability of arsenic sulfides is great enough to preclude a larger abundance of gaseous arsenic compounds irrespective of the crustal abundance of arsenic. The same may be true of antimony, since the mineral Sb_2S_3 seems to have low enough volatility to hide antimony in the lithosphere. We have also briefly considered bismuth, and find that Bi_2S_3 is so stable that the most abundant bismuth-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 are in error.

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21. The pressure, temperature, composition conditions assumed in these calculations are 95 bars total pressure, 750 K surface temperature, $P_{O_2} = 10^{-22.5}$ bar, $P_{HCl} = 10^{-4.0}$ bar, $P_{S_2} = 10^{-4.0}$ bar, and $P_{HF} = 10^{-5.2}$ bar.
22. Other As- and Sb-bearing gases included in the calculations but not abundant enough to be graphed are As, AsO, AsH_3, AsF, AsF_2, AsF_3, AsF_5, AsCl, $AsCl_2$, $AsCl_3$, Sb, SbO, SbH_3, SbN, and SbF_3. The solid and liquid arsenic oxides As_2O_4, As_2O_5, and As_4O_6 are unstable and do not precipitate as pure condensates on the surface of Venus. Formation of more complex minerals, such as 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.

23. 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 G. K. Johnson for providing his Sb_2S_3 data before publication. B.F. also thanks A. G. W. Cameron for support and facilities.

23 November 1981; revised 30 March 1982

III

Shock-Wave Processing of Interstellar Cloud Materials

Prior to the discovery of the short-lived radinuclide aluminum-26 in meteorite inclusions by Lee, et al. (1973), the evolution of the presolar nebula was commonly assumed to have taken place in isolation from astrophysical disturbing forces. However, the necessity of having active nucleosynthesis ocurring virtually simultaneously with the collapse of the presolar nebula strongly suggests that there is more than mere coincidence at work here. It is, in fact, entirely plausible to believe that the collapse of the nebula was triggered by a nearby supernova explosion. It has become well established that most supernovae occur in star-forming regions: indeed, it is hard to see how it could be otherwise, since the lifetimes of the massive stars responsible for supernova explosions are comparable to or shorter than the lifetimes of the dense molecular cloud complexes that give rise to stars. It is obviously important to understand how the chemical and physical evolution of dense clouds are influenced by nearby supernova explosions.

We consider here the effects of brief, intense shock events on interstellar clouds with pressures of 10^-10 b or higher; that is, in the densest molecular cloud regions. These regions are most vulnerable to external disturbances, and most likely to be triggered into rapid collapse by a shock event. We take the initial temperature to be 90K, well below the saturation point of ice. Shock heating is relatively ineffectual at heating the solid ice grains, and the release of water vapor into the gas will be incomplete and inhomogeneous at best. The models reported herein assume a 10^4-fold depletion of oxygen relative to carbon in the gas; however, very similar results are found for runs in which the oxygen depletion is only a factor of two.

The results for a number of interesting products are shown in Fig. 1. Note that the abundances of most of the complex molecular products grow rapidly with increasing pressure along the 2000K isotherm. This is not solely a pressure effect, however, since cooling the low-pressure runs to 1800 or 1600 K also gives a large yield of products. It is irrelevant whether the peak shock temperature is too high for optimum yields of complex products (as it clearly is in the low-pressure 2000K runs), since post-shock cooling through more benign temperatures will form these products without any memory of prior, higher-temperature conditions.

A number of features of these results are of interest. First, the dominant carbon compound at high temperatures and low pressures, atomic C (Lewis, et al., 1979) forms HCN, C2H and C2H2 very efficiently at slightly lower temperatures. This was documented for C novae by Lewis and Ney (1979).

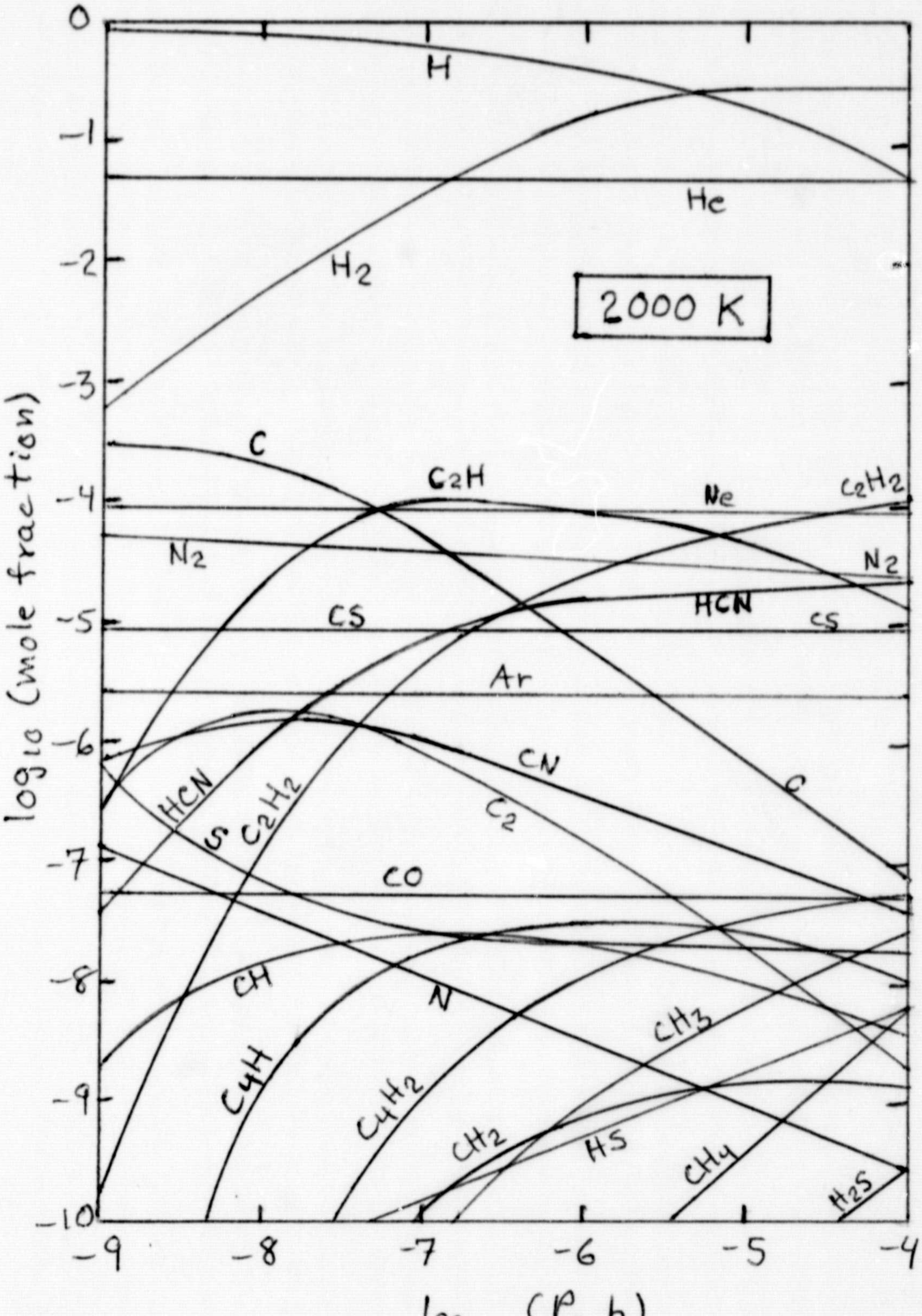
Note also that, in any C-rich system, oxygen is essentially completely tied up as CO. The multiple-bonded molecules CN, C2, CO, CS and N2 are quite abundant. In analogy with the behavior of oxygen, sulfur is essentially all carried by CS.

Quenching and further slow cooling of the gas mixtures described herein would surely lead to spontaneous polymerization of HCN, C2H and C2H2 on grain surfaces. Because of the paucity of oxygen in the gas (due to the very cold initial temperatures of interstellar dense clouds), essentially no water-soluble organics (alcohols, acids, ketones, aldehydes, esters, amino acids, etc.)

Caption to Fig. 1.

Mole fractions of gases in an interstellar cloud shocked to 2000K, as a function of the peak shock pressure. For lower temperatures the general behavior is similar, but the abundance curves are shifted to the left.

Fig. 1


0
-1
-2
-3
-4
-5
-6
-7
-8
-9
-10
-9
-8
-7
-6
-5
-4
log10 (mole fraction)
log10 (P, b)
2000 K
H
He
H2
C
C2H
Ne
C2H2
N2
N2
HCN
CS
CS
Ar
CN
C
C2
HCN
S
C2H2
CO
CH
N
CH3
C4H
C4H2
CH2
HS
CH4
H2S

are formed.

Throughout the regime explored, ammonia is a very minor constituent. Thus ammonia, its salts, and organic amines are very minor products from shock heating events.

Conditions conducive to the formation of complex polymeric organic matter, essentially devoid of soluble organic species, should be found in C-nova ejecta, in shocked interstellar clouds, and in shocked regions of the solar nebula in which water is largely condensed prior to the shock.

It will be easy to follow up on these results by modeling the chemical consequences of shock processing of solar nebular material originating both above and below the ice saturation point. Plausible sources of shock energy include supersonic accretion of interstellar material onto the nebular disc, bow shocks in front of massive accreting planetesimals that have attained Keplerian speeds, and lightning produced by charge-separation effects in the turbulent, dusty nebular gas. Cameron's time-dependent accretion disc models permit a reasonable approximate quantification of the first effect, and the latter, based on an old suggestion by Whipple, can be reasonably treated using recent results on the efficiency of lightning production by convective energy fluxes on Venus, Earth, and Jupiter.

The continuation of this project at the University of Arizona, which will be based on computer programs now fully developed under the present grant, will be able to produce publishable work on isolated-grain condensation, on the shock-wave chemistry of star-forming regions, and on the shock chemistry of the solar nebula. Much of the computer work for these projects has already been done.

```
1 REM '                    PROGRAM gashock
2'REM        best first-guess; 35/65; 470 ITER>12
10 READ BH, BHE, BO, BC, BN, BSU, BNE, BAR
20 FOR NT = 1 TO 10
25 READ T, KH, KH2O, KCO, KCH4, KCO2
26 READ T, KOH, KO, KC, KH2S, KHS
27 READ T, KCN, KHCN, KNH3, KSO2, KS
33 READ T, KC2, KC2H, KC2H2, KC3H4AC, KN
34 READ T, KC3H4AL, KC3H6, KC3H8, KC2H6, KC2H4
35 READ T, KC4, KC4H, KC4H2, KCH3NH2, KCH3SH
36 READ T, KCH3CN, KC2N2, KCH, KCH2
37 READ T, KCH3, KCHO, KCH2O, KNH
38 READ T, KNH2, KCS, KCOS, KCS2, KHCNO
39 READ T, KCH3OH, KHCOOH, KN2H4
50 FOR NP = 1 TO 10
59 F = 10^(NP-13)
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
72 ABAR = F*BAR
80 REM INITIAL GUESS OF ELEMENTAL ACTIVITIES
81 RH = (-KH+SQR(KH^2+8*ABH))/4
82 RN = (-KN+SQR(KN^2+8*ABN))/4
83 PH2 = RH^2
84 RO = (2*ABO)/(3*KH2O*PH2)
85 GR = ABC/((KCO*RO)+(KCH4*PH2^2))
86 RS = ABSU/((KSO2*RO^2)+(KH2S*PH2))
87 IF ABC>ABO THEN 88 ELSE 99
88 A = KC2H*RH + KC2H2*PH2
89 B = KC + KCH4*PH2^2
91 GR = (-B+SQR(B^2+4*A*ABC))/(2*A)
92 RO = ABO/(KCO*GR+KH2O*PH2O)
93 RS = ABSU/(KSO2*RO^2+KH2S*PH2+KCS*GR)
94 BB = KHCN*GR*RH + KN
95 RN = (-BB+SQR(BB^2+4*ABN))/2
99 INDEX = 0
100 PRINT "ITER","INDEX","ABO/SO","ABN/SN","Graphite"
200 FOR ITER = 1 TO 150
201 INDEX = INDEX+1
202 PH = KH*RH
203 PH2 = RH^2
204 PHE = ABHE
205 PNE = ABNE
206 PAR = ABAR
207 PC2 = KC2*GR^2
208 PC2H = KC2H*RH*GR^2
209 PC2H2 = KC2H2*PH2*GR^2
210 PCO = KCO*GR*RO
211 PCH4 = KCH4*GR*PH2^2
212 PCO2 = KCO2*RO*GR*RO
213 PC = KC*GR
214 PC3H4AC = KC3H4AC*PH2^2*GR^3
215 PC3H4AL = KC3H4AL*PH2^2*GR^3
216 PC3H6 = KC3H6*(PH2*GR)^3
217 PC3H8 = KC3H8*PH2*(PH2*GR)^3
218 PC4 = KC4*GR^4
219 PC4H = KC4H*RH*GR^4
220 POH = KOH*RH*RO
221 PH2O = KH2O*PH2*RO
222 PO = KO*RO
223 PO2 = PO^2
```

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224 PC4H2 = KC4H2*PH2*GR^4
225 PCH3CN = KCH3CN*RN*GR^2*PH2*RH
226 PC2N2 = KC2N2*PN2*GR^2
227 PCH = KCH*GR*RH
228 PCH2 = KCH2*GR*PH2
229 PCH3 = KCH3*GR*PH2*RH
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
235 PCHO = KCHO*GR*RH*RO
236 PCH2O = KCH2O*GR*PH2^RO
237 PNH = KNH*RN*RH
238 PNH2 = KNH2*RN*PH2
239 PCS = KCS*GR*RS
240 PH2S = KH2S*RS*PH2
241 PSO2 = KSO2*RS*PO2
242 PHS = KHS*RH*RS
243 PS = KS*RS
244 PS2 = RS^2
245 PCOS = KCOS*GR*RO*RS
246 PCS2 = KCS2*GR*PS2
247 PHCNO = KHCNO*RH*GR*RN*RO
248 PC2H6 = KC2H6*GR^2*PH2^3
249 PC2H4 = KC2H4*GR^2*PH2^2
250 PCH3NH2 = KCH3NH2*GR*RN*RH*PH2^2
251 PCH3SH = KCH3SH*GR*RS*PH2^2
252 PCH3OH = KCH3OH*GR*RO*PH2^2
253 PHCOOH = KHCOOH*GR*PO2*PH2
254 PN2H4 = KN2H4*PN2*PH2^2
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+PHCNO+PCS2+PCOS+PCS+PCHO+PCH2O+PCH+PCH2+PCH3+
2*(PC2N2+PCH3CN+PC2+PC2H+PC2H2)+3*(PC3H4AC+PC3H4AL+PC3H6+PC3H8)+4*(PC4+PC4H+PC4H
2)
403 SO = PH2O+2*PO2+2*PCO2+PCO+POH+2*PSO2+PO+PCHO+PCH2O+PCOS+PHCNO
404 SN = PN+2*PN2+PNH3+PCN+PHCN+PCH3CN+PNH+PNH2+PHCNO+2*PC2N2
405 SS = PS+PHS+PSO2+PH2S+2*PS2+PCS+PCOS+PCS2
419 P = PH2+PH+PH2O+PCO+PCO2+PCH4+PN2+PNH3+POH+PH2S+PHE+PO+PNE+PHS+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-ABSU)/ABSU
429 PRINT ITER, INDEX, ABO/SO; ABN/SN; GR
430 IF EH<.001 THEN IF EO<.001 THEN IF EC<.001 THEN IF EN<.001 THEN IF ES<.001 T
HEN GOTO 501 ELSE 431
431 RHNEW = RH
432 RONEW = RO
433 RNNEW = RN
434 RSNEW = RS
435 GRNEW = GR
440 IF INDEX = 1 THEN 444 ELSE 455
444 IF PH>PH2 THEN 445 ELSE 452
445 RHNEW = RH*(ABH/SH)
446 GOTO 470
452 RHNEW = RH*SQR(ABH/SH)
453 GOTO 470
455 IF INDEX = 2 THEN 456 ELSE 462
456 RNNEW = RN*SQR(ABN/SN)
457 RONEW = RO*(ABO/SO)
459 GOTO 470
462 GRNEW = GR*(ABC/SC)
465 RSNEW = RS*(ABSU/SS)
466 INDEX = 0
```

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```
450 INDEX = 0
470 IF ITER<12 THEN 471 ELSE 481
471 RH = RHNEW
472 RO = RONEW
473 RN = RNNEW
474 GR = GRNEW
475 RS = RSNEW
476 GOTO 500
481 RH = .35*RH+.65*RHNEW
482 RO = .35*RO+.65*RONEW
483 RN = .35*RN+.65*RNNEW
484 RS = .35*RS+.65*RSNEW
485 GR = .35*GR+.65*GRNEW
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
509 PRINT "O =";PO;" O2 =";PO2;" OH =";POH;"  H2O =";PH2O
510 PRINT "N =";PN;" N2 =";PN2;" NH3 =";PNH3;" CN =";PCN;" N2H4 =";PN2H4
511 PRINT "C =";PC;" CO =";PCO;" CO2 =";PCO2;" CH4 =";PCH4;"HCN =";PHCN;"SO2 =";
PSO2;" Ar =";PAR
512 PRINT "S =";PS;" S2 =";PS2;" HS =";PHS;" H2S =";PH2S
515 PRINT "C2 =";PC2;" C2H =";PC2H;" C2H2 =";PC2H2;" CH2CCH2 =";PC3H4AL;" CH3CCH
 =";PC3H4AC;" C3H8 =";PC3H8;" C4 =";PC4
516 PRINT "C4H =";PC4H;" C4H2 =";PC4H2;" CH3C2H =";PCH3C2H;" CH3CN =";PCH3CN;" C
2N2 =";PC2N2;" CH =";PCH;" CH2 =";PCH2
517 PRINT " CH3 =";PCH3;" CHO =";PCHO;" CH2O =";PCH2O;" NH =";PNH;" NH2 =";PNH2;
" CS =";PCS;" CH3OH =";PCH3OH
518 PRINT "CS2 =";PCS2;" HCNO =";PHCNO;" C2H6 =";PC2H6;" C2H4 =";PC2H4;" CH3NH2
=";PCH3NH2;" CH3SH =";PCH3SH;" HCOOH =";PHCOOH
535 PRINT "      Input Abundances of Elements"
536 PRINT "H =";ABH;" O =";ABO;" C =";ABC;" N =";ABN;" S =";ABSU
538 PRINT "      Calculated Abundances of Elements        Graphite Activity =";GR

539 PRINT "H =";SH;" O =";SO;" C =";SC;" N =";SN;" S =";SS
545 INPUT "Input (1) to go on; (0) to end: ",GOON
546 IF GOON = 1 THEN 590 ELSE 650
590 NEXT NP
600 NEXT NT
610 DATA 1756.,122.,1.192e-4,0.6516,0.2065,0.0221,0.2295,6.222E-3
625 DATA 2000, 1.622E-3, 3467.4, 2.944E7, 3.908E-4, 2.254E10
626 DATA 2000, 0.5808, 6.637E-4, 3.342E-11, 0.614, 0.1033
627 DATA 2000, 2.183E-7, 1.472E-2, 2.046E-5, 4.498E5, 2.871E-3
633 DATA 2000, 1.611E-12, 1.714E-6, 8.81E-4, 5.026E-8, 9.5E-10
634 DATA 2000, 2E-8, 2.884E-10, 5.75E-14, 7.063E-9, 1.121E-5
635 DATA 2000, 2.838E-15, 3E-9, 1.6E-6, 6.683E-11, 5.408E-7
636 DATA 2000, 9.736E-7, 1.61E-6, 2.01E-10, 9.099E-9
637 DATA 2000, 1.556E-5, 442.6, 19.28, 2.446E-8
638 DATA 2000, 1.706E-7, 2.286, 6.592E5, 4.227, 15.07
639 DATA 2000, 3.289E-3, 3.674E4, 5.768E-15
650 END
```

```
 22          1              .9998351  .9999986  1.875164E-02
Temperature =  2000 .        Pressure =  1.877169E-09     22 Iterations
         Pressures of Gases in Bars
H = 1.753662E-09  H2 = 1.168934E-12  He = 1.22E-10  Ne = 2.295E-13
O = 1.433318E-25  O2 = 0  OH = 1.356102E-28   H2O = 8.753159E-31
N = 3.039932E-16  N2 = 1.023955E-13  NH3 = 8.274296E-30  CN = 1.309885E-15
 N2H4 = 0
C = 6.266797E-13  CO = 1.192197E-16  CO2 = 1.971218E-35  CH4 = 1.001322E-29
HCN = 9.549538E-17 SO2 = 0  Ar = 6.222E-15
S = 1.396518E-15  S2 = 2.333441E-25  HS = 5.395029E-20  H2S = 3.467025E-25
C2 = 5.66466E-16  C2H = 6.516047E-16  C2H2 = 3.621131E-19  CH2CCH2 =
 1.801887E-37  CH3CCH = 4.528143E-37  C3H8 = 0  C4 = 3.508885E-22
C4H = 4.010264E-22  C4H2 = 2.31242E-25  CH3C2H = 0  CH3CN = 1.384472E-34  C2N2 =
 5.796754E-23  CH = 4.075025E-18  CH2 = 1.994449E-22
 CH3 = 3.687515E-25  CHO = 1.937834E-27  CH2O = 0  NH = 8.462368E-21  NH2 =
 6.381304E-26  CS = 2.070684E-14  CH3OH = 0
CS2 = 1.84956E-26  HCNO = 2.111342E-35  C2H6 = 0  C2H4 = 5.385972E-33  CH3NH2 =
 0  CH3SH = 0  HCOOH = 0
     Input Abundances of Elements
H = 1.756E-09  O = 1.192E-16  C = 6.516E-13  N = 2.065E-13  S = 2.21E-14
     Calculated Abundances of Elements        Graphite Activity = 1.875164E-02
H = 1.756E-09  O = 1.192197E-16  C = 6.51352E-13  N = 2.065003E-13  S =
 2.210341E-14
Input (1) to go on; (0) to end:
1LIST   2RUN  3LOAD"  4SAVE"  5CONT 6,"LPT1 7TRON 8TROFF9KEY    0SCREEN

 30          3              .9995598  .9999872  .1570265
Temperature =  2000          Pressure =  1.866916E-08     30 Iterations
         Pressures of Gases in Bars
H = 1.733162E-08  H2 = 1.141765E-10  He = 1.22E-09  Ne = 2.295E-12
O = 1.712098E-25  O2 = 0  OH = 1.600928E-27   H2O = 1.021263E-28
N = 9.511923E-16  N2 = 1.002512E-12  NH3 = 2.499283E-26  CN = 3.43219E-14
 N2H4 = 0
C = 5.247824E-12  CO = 1.192525E-15  CO2 = 2.355268E-34  CH4 = 7.999832E-25
HCN = 2.472941E-14 SO2 = 0  Ar = 6.222E-14
S = 1.766626E-15  S2 = 3.734162E-25  HS = 6.745051E-19  H2S = 4.283924E-23
C2 = 3.972293E-14  C2H = 4.515906E-13  C2H2 = 2.480267E-15  CH2CCH2 =
 1.00949E-30  CH3CCH = 2.536848E-30  C3H8 = 0  C4 = 1.725456E-18
C4H = 1.948952E-17  C4H2 = 1.110678E-19  CH3C2H = 0  CH3CN = 2.932487E-29
 C2N2 = 3.979949E-20  CH = 3.372541E-16  CH2 = 1.631335E-19
 CH3 = 2.980901E-21  CHO = 1.915709E-25  CH2O = 0  NH = 2.616915E-19  NH2 =
 1.950296E-23  CS = 2.193541E-13  CH3OH = 0
CS2 = 2.478554E-25  HCNO = 6.530945E-33  C2H6 = 0  C2H4 = 3.603337E-27  CH3NH2 =
 0  CH3SH = 0  HCOOH = 0
     Input Abundances of Elements
H = 1.756E-08  O = 1.192E-15  C = 6.516E-12  N = 2.065E-12  S = 2.21E-13
     Calculated Abundances of Elements        Graphite Activity = .1570265
H = 1.756E-08  O = 1.192525E-15  C = 6.515433E-12  N = 2.065026E-12  S =
 2.211214E-13
Input (1) to go on; (0) to end:
1LIST   2RUN  3LOAD"  4SAVE"  5CONT 6,"LPT1 7TRON 8TROFF9KEY    0SCREEN
```

```
 40             1               1.000858  1.000078  .3718258
Temperature =  2000          Pressure =  1.784758E-07      40 Iterations
        Pressures of Gases in Bars
H = 1.568871E-07  H2 = 9.355629E-09  He = 1.22E-08  Ne = 2.295E-11
O = 7.221016E-25  O2 = 0  OH = 6.112088E-26   H2O = 3.529421E-26
N = 2.910689E-15  N2 = 9.387379E-12  NH3 = 5.672667E-23  CN = 2.486941E-13
 N2H4 = 0
C = 1.242642E-11  CO = 1.190978E-14  CO2 = 9.920794E-33  CH4 = 1.271862E-20
HCN = 1.622019E-12 SO2 = 0  Ar = 6.222E-13
S = 7.48362E-15  S2 = 6.70081E-24  HS = 2.586428E-17  H2S = 1.48698E-20
C2 = 2.227279E-13  C2H = 2.292062E-11  C2H2 = 1.139536E-12  CH2CCH2 =
 8.999006E-26  CH3CCH = 2.261451E-25  C3H8 = 0  C4 = 5.424635E-17
C4H = 5.54646E-15  C4H2 = 2.861219E-16  CH3C2H = 0  CH3CN = 3.731997E-25  C2N2 =
 2.089533E-18  CH = 7.228898E-15  CH2 = 3.165237E-17
 CH3 = 5.235505E-18  CHO = 1.731865E-23  CH2O = 0  NH = 7.248784E-18  NH2 =
 4.890173E-21  CS = 2.200287E-12  CH3OH = 0
CS2 = 1.053172E-23  HCNO = 1.806708E-30  C2H6 = 7.996268E-34  C2H4 =
 1.356534E-22  CH3NH2 = 6.445635E-37  CH3SH = 4.556023E-35  HCOOH = 0
    Input Abundances of Elements
H = 1.756E-07  O = 1.192E-14  C = 6.516001E-11  N = 2.065E-11  S = 2.21E-12
    Calculated Abundances of Elements          Graphite Activity = .3718258
H = 1.756E-07  O = 1.190978E-14  C = 6.510593E-11  N = 2.064839E-11  S =
 2.207797E-12
Input (1) to go on; (0) to end:
1LIST   2RUN  3LOAD"  4SAVE"  5CONT 6,"LPT1 7TRON 8TROFF9KEY    0SCREEN

 49             1               .9992615  .9998802  .4549451
Temperature =  2000          Pressure =  1.49946E-06       49 Iterations
        Pressures of Gases in Bars
H = 9.983176E-07  H2 = 3.788225E-07  He = 1.22E-07  Ne = 2.295E-10
O = 5.911151E-24  O2 = 0  OH = 3.183792E-24   H2O = 1.169876E-23
N = 8.702916E-15  N2 = 8.392328E-11  NH3 = 4.370191E-20  CN = 9.098168E-13
 N2H4 = 6.946709E-38
C = 1.520427E-11  CO = 1.192881E-13  CO2 = 8.134173E-31  CH4 = 2.551438E-17
HCN = 3.775947E-11 SO2 = 0  Ar = 6.222E-12
S = 6.130428E-14  S2 = 4.496612E-22  HS = 1.34822E-15  H2S = 4.93227E-18
C2 = 3.334368E-13  C2H = 2.183467E-10  C2H2 = 6.90764E-11  CH2CCH2 =
 2.702579E-22  CH3CCH = 6.791581E-22  C3H8 = 0  C4 = 1.215762E-16
C4H = 7.909975E-14  C4H2 = 2.59652E-14  CH3C2H = 0  CH3CN = 4.304208E-22  C2N2 =
 2.796574E-17  CH = 5.628244E-14  CH2 = 1.568153E-15
 CH3 = 1.650525E-15  CHO = 1.103795E-21  CH2O = 0  NH = 1.379163E-16  NH2 =
 5.920467E-19  CS = 2.205352E-11  CH3OH = 1.91247E-36
CS2 = 8.647224E-22  HCNO = 3.442956E-28  C2H6 = 7.947204E-29  C2H4 =
 3.329623E-19  CH3NH2 = 2.460146E-32  CH3SH = 7.487034E-31  HCOOH = 0
    Input Abundances of Elements
H = 1.756E-06  O = 1.192E-13  C = 6.516E-10  N = 2.065E-10  S = 2.21E-11
    Calculated Abundances of Elements          Graphite Activity = .4549451
H = 1.756E-06  O = 1.192881E-13  C = 6.520398E-10  N = 2.065247E-10  S =
 2.211618E-11
Input (1) to go on; (0) to end:
1LIST   2RUN  3LOAD"  4SAVE"  5CONT 6,"LPT1 7TRON 8TROFF9KEY    0SCREEN
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 49            1   .9994402  .9998721  .5264224
Temperature =  2000          Pressure =  1.209942E-05     49 Iterations
         Pressures of Gases in Bars
H = 4.193159E-06  H2 = 6.683144E-06  He = 1.22E-06  Ne = 2.295E-09
O = 5.107626E-23  O2 = 5.922356E-39  OH = 1.155485E-22   H2O = 1.783331E-21
N = 2.61154E-14  N2 = 7.556942E-10  NH3 = 9.717395E-18  CN = 3.159084E-12
 N2H4 = 1.946852E-34
C = 1.759304E-11  CO = 1.192668E-12  CO2 = 7.0272[illegible]-29  CH4 = 9.188626E-15
HCN = 5.50688E-10 SO2 = 0  Ar = 6.222E-11
S = 5.298232E-13  S2 = 3.358657E-20  HS = 4.894109E-14  H2S = 7.520246E-16
C2 = 4.464412E-13  C2H = 1.22792E-09  C2H2 = 1.631644E-09  CH2CCH2 =
 1.303151E-19  CH3CCH = 3.274818E-19  C3H8 = 1.673378E-35  C4 = 2.179465E-16
C4H = 5.955922E-13  C4H2 = 8.211797E-13  CH3C2H = 0  CH3CN = 1.281426E-19
 C2N2 = 3.371636E-16  CH = 2.7354E-13  CH2 = 3.20117E-14
 CH3 = 1.415191E-13  CHO = 4.63536E-20  CH2O = 0  NH = 1.738281E-15  NH2 =
 3.134245E-17  CS = 2.205431E-10  CH3OH = 5.951235E-33
CS2 = 7.473643E-20  HCNO = 4.338687E-26  C2H6 = 5.842522E-25  C2H4 =
 1.387509E-16  CH3NH2 = 1.116686E-28  CH3SH = 2.33032E-27  HCOOH = 0
     Input Abundances of Elements
H = 1.756E-05  O = 1.192E-12  C = 6.516E-09  N = 2.065E-09  S = 2.21E-10
     Calculated Abundances of Elements        Graphite Activity = .5264224
H = 1.756E-05  O = 1.192668E-12  C = 6.519321E-09  N = 2.065264E-09  S =
 2.211226E-10
Input (1) to go on; (0) to end:
1LIST   2RUN  3LOAD"  4SAVE"  5CONT 6,"LPT1 7TRON 8TROFF9KEY    0SCREEN

Temperature =  2000          Pressure =  1.073048E-04     43 Iterations
         Pressures of Gases in Bars
H = 1.455464E-05  H2 = 8.051949E-05  He = .0000122  Ne = 2.295E-08
O = 4.701451E-22  O2 = 5.017879E-37  OH = 3.691792E-21   H2O = 1.977721E-19
N = 8.022649E-14  N2 = 7.131623E-09  NH3 = 1.248393E-15  CN = 1.05473E-11
 N2H4 = 2.666955E-31
C = 1.912052E-11  CO = 1.19314E-11  CO2 = 6.470941E-27  CH4 = 1.449606E-12 HCN =
 6.381839E-09 SO2 = 0  Ar = 6.222E-10
S = 4.875208E-12  S2 = 2.843741E-18  HS = 1.563133E-12  H2S = 8.337089E-14
C2 = 5.273297E-13  C2H = 5.034403E-09  C2H2 = 2.322007E-08  CH2CCH2 =
 2.428354E-17  CH3CCH = 6.102453E-17  C3H8 = 4.526389E-31  C4 = 3.040785E-16
C4H = 2.884331E-12  C4H2 = 1.380366E-11  CH3C2H = 0  CH3CN = 1.944522E-17
 C2N2 = 3.758382E-15  CH = 1.031905E-12  CH2 = 4.191679E-13
 CH3 = 6.432124E-12  CHO = 1.60959E-18  CH2O = 0  NH = 1.853537E-14  NH2 =
 1.160043E-15  CS = 2.205538E-09  CH3OH = 8.6421E-30
CS2 = 6.877263E-18  HCNO = 4.628192E-24  C2H6 = 1.206921E-21  C2H4 =
 2.378999E-14  CH3NH2 = 1.878501E-25  CH3SH = 3.382805E-24  HCOOH =
 8.492854E-37
     Input Abundances of Elements
H = .0001756  O = 1.192E-11  C = 6.516E-08  N = 2.065E-08  S = 2.21E-09
     Calculated Abundances of Elements        Graphite Activity = .5721282
H = .0001756  O = 1.19314E-11  C = 6.521508E-08  N = 2.065574E-08  S =
 2.21206E-09
Input (1) to go on; (0) to end:
1LIST   2RUN  3LOAD"  4SAVE"  5CONT 6,"LPT1 7TRON 8TROFF9KEY    0SCREEN
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