Equilibrium Concentrations
of N_2H_4 and its Decomposition Products
at Elevated Temperatures and Pressures

by

Frederick O. Smetana

Howard N. Fairchild II

Glenn L. Martin

Department of Mechanical and Aerospace Engineering
School of Engineering
North Carolina State University
Raleigh, North Carolina

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INTRODUCTION

Increasingly, liquid hydrazine (N_2H_4) is coming to be considered as a convenient source of hydrogen rather than just as a rocket fuel. For such purposes, the hydrogen is usually obtained by passing the hydrazine through a heated catalytic bed. One convenient measure of the effectiveness of a catalytic decomposition device as a whole is to compare the quantity of hydrogen produced with the equilibrium concentration of the gaseous species N_2H_4, NH_3, N_2, and H_2 which would exist at the temperature and pressure found in various parts of the device. Since such data do not seem to be readily available in the literature, calculations of the concentrations were carried out and are reported here.

The report begins with a review of the pertinant literature, citing experimental results or curve fits to the data where available. The basis for the computer program is then described. Following presentation of the results in both tabular and graphical forms is a comparison between the computed equilibrium concentrations and available experimental data.

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SURVEY OF THE LITERATURE

This section provides a brief survey of the available literature on the thermodynamic properties of hydrazine and its decomposition products as well as the decomposition reaction itself.

Several surveys of the thermodynamic properties of hydrogen, nitrogen, ammonia, and hydrazine are available in the literature. The first of these, by J. B. Evans and V. J. DeCarlo (1965) was intended as a bibliography for investigations into the chemistry of "cometary phenomena". A second bibliography of thermo-chemical data was published by M. K. Buresh, M. L. Reilly, G. T. Furukawa, and G. T. Armstrong (1965) of the National Bureau of Standards. This particular report listed the low-range temperature range data for the heat-capacities, enthalpy, and entropy of ammonia, carbon dioxide, and water. Both reports consisted of references to other investigations. Properties of gaseous nitrogen, hydrogen, ammonia, and hydrazine have been tabulated and are presented graphically in the N.A.S.A. Design Guide for Pressurized Gas Systems, Volume II (1966).

The data for hydrogen and nitrogen are well known and will therefore not be discussed further here.

J. L. Haws and D. G. Harden (1965) presented empirical equations for the thermodynamic properties of hydrazine, including vapor pressure, saturated liquid density, and the heat capacities. From the 'triple point' to the critical point, the vapor pressure is represented by

$$(1)\quad \ell n\,P = 24.24 - (18{,}184.9/T) + 0.47629(\ell n\,T) - 0.003863T +$$

$$(1115.43(1190.08 - T)/1190.088)\ell n(1190.8 - T)$$

for pressure in psia units and temperature in °R units. The error is relatively small. For the heat capacities, these authors give the following relations:

$$(2)\quad C_p = 0.137858 + 0.052715 \times 10^{-3}T - 0.119907 \times 10^{-6}T^2$$

$$(3)\quad C_v = 0.075903 + 0.52715 \times 10^{-3}T - 0.119907 \times 10^{-3}T^3$$

An equation of state for gaseous hydrazine was presented in the form

$$(4)\quad P = RT/(V - b) + \frac{A_2 + B_2T + C_2e^{-xT/T_c}}{(V - b)^2} + \frac{A_3 + B_3T + C_3e^{-xT/T_c}}{(V - b)^3} + \frac{A_4}{(V - b)^4} + \frac{B_5T}{(V - b)^5}$$

where $R = 10.7315/\text{mole wt}$

$b = 0.0299451\ \text{ft}^3/\text{lbm}$

$x = 8.0000$

$T_c = 1175.69°\text{R}$

$A_2 = -32.21898$

$B_2 = 0.00294549$

$C_2 = -1171.2876$

$A_3 = 0.869588$

$B_3 = 0.16838487 \times 10^{-3}$

$C_3 = 46.250721$

$A_4 = -0.202100 \times 10^{-1}$

$B_5 = 0.12899897 \times 10^{-6}$

The equations were used in computing property values for a temperature range from 32 °F to 1400°F, and for pressures from 1.0 psia to 8000 psia. It should be noted that the equations were curve-fitted to match experimental data provided by other investigators.

M. S. Jhon, J. Grosh, and H. Eyring (1967), using the significant structure theory of liquids, computed the thermodynamic properties of liquid hydrazine (and other chemicals). The computational results were claimed to be in good agreement with experimentally-determined property data. These properties were 1) the vapor pressure, 2) the molar volume, 3) the entropy, 4) the critical temperature and pressure, 5) the constant volume and constant pressure heat capacities, 6) the coefficient of thermal expansion, and 7) the compressibility. The surface tension and the dielectric constant were computed by other methods which are related to the significant structure theory of liquids.

The "significant structure" theory for liquids is actually a model approach for describing the mechanical and thermodynamic properties of liquids.

Let V be the mole volume of the liquid state, V_s be the mole volume of the solid state at the melting point, and V_o be the mole volume of the "solidlike structure" in its molten state. The "excess volume" of the liquid is defined as $V - V_s$. This volume is due to expansion of the chemical substance upon melting and entering the liquid phase. The liquid is considered to have molecular "vacancies" in its interior, and the total volume of these vacancies is the "excess volume". This volume permits molecules in the liquid state to have translational degrees of freedom.

If a molecule is completely surrounded by other molecules, then it can only oscillate. The oscillation frequency will be nearly the same as if the molecule were in a solid state. If the molecule is adjacent to a "vacancy", then the molecule will have translational degrees of freedom, and will behave as if it were in a gaseous phase.

The partition function used in the theory is formed from the multiplication of the partition functions for each type of structure. A factorial term is included to account for the lack of distinction between the 'gas' molecules.

The liquid state partition function was written in the form

$$(5) \qquad f = \frac{\left[f_{\text{solid}}\, f_{\text{deg}}\right]^{\frac{NV_o}{V}} \left[f_{\text{gas}}\right]^{\frac{N(V - V_o)}{V}}}{\left[\frac{N(V - V_o)}{V}\right]!}$$

where $f_{(\ )}$ are the partition functions for solid and gas states, and the molecular degeneracy of position.

The Helmholtz free energy function was expressed as

$$(6) \qquad A = -kT \ln (f).$$

Using the above equation, the vapor pressure was computed in the following manner. For a constant temperature, the Helmholtz free energy was plotted as a function of volume. Through points common to the liquid and vapor states, a tangent was drawn, whose slope gives the vapor pressure. The values of volume for the two tangency points give the values for the liquid and vapor molar volumes.

The entropy of vaporization was computed from the relation

$$(7) \qquad S = -\left[\frac{\partial A}{\partial T}\right]_V = \left[\frac{\partial}{\partial T}(kT \ln f)\right]_V$$

and the vaporization entropy was given by $S_g - S_l$, where 'g' and 'l' indicate vapor and liquid states respectively. The constant-volume heat capacity is given by

$$(8) \qquad C_V = \frac{\partial}{\partial T}\left[kT^2 \frac{\partial \ln f}{\partial T}\right]_V$$

and the constant-pressure heat-capacity is given by

$$(9) \qquad C_p = C_V + TV\frac{\alpha^2}{\beta}$$

where

$$(10) \qquad \alpha = \frac{1}{V}\left[\frac{\partial V}{\partial T}\right]_P = -\frac{1}{V}\left[\frac{\partial^2 A}{\partial V \partial T}\right]_{TV} \Big/ \left[\frac{\partial^2 A}{\partial V^2}\right]_T$$

which is the thermal expansion coefficient, and

$$(11) \qquad \beta = -\frac{1}{V}\left[\frac{\partial V}{\partial P}\right]_T = 1 \Big/ V\left[\frac{\partial^2 A}{\partial V^2}\right]_T$$

which is the compressibility. The critical temperature, pressure, and volume were computed by an iteration method using the conditions

(12) $$\left.\frac{\partial P}{\partial V}\right|_T = 0$$

(13) $$\left.\frac{\partial^2 P}{\partial V^2}\right|_T = 0$$

(14) $$P = -\left[\frac{\partial A}{\partial V}\right]_T$$

The surface tension was computed by an iteration technique which accounted for polar liquid orientation effects. The dielectric constant was expressed as a function of the index of refraction and the dipole moment.

A comparison of the results of Haws and Harden, with those of Jhon, Grosh, and Eyring, for vapor pressure and constant pressure heat capacity show discrepancies. Only for the saturated liquid density is there reasonable agreement. The following table compares the results of the two computations for the vapor pressure of N_2H_4.

Table I. Comparison of computed vapor pressures.

T, °K	P, atm(Haws and Harden)	P, atm(Jhon *et al.*)
273	0.003539	0
293	0.0135658	0.01
313	0.04322	0.04
333	0.11850	0.20
343	0.18696	0.27

No comparison is possible for temperatures above 400 °K.

A comparison of the constant-pressure heat capacities gives the following:

Table 2. Comparison of computed constant-pressure heat capacities.

T, °K	c_p, cal/g-mole-°K (Haws and Harden)	c_p, cal/g-mole-°K (Jhon et al.)
273	11.7792	20.84
298	12.3854	21.27
300	12.4064	21.35
400	14.5728	25.575

The comparison of results for both vapor pressure and constant-pressure heat-capacities show that Jhon, Grosh, and Eyring consistently obtained higher values at elevated temperatures than did Haws and Harden.

By contrast, the results obtained in each study for the saturated liquid density were in good agreement.

Table 3. Comparison of computed specific volumes.

T, °K	V, cc/mole (H&H)	V, cc/mole (J,G,&E)
273	31.261	31.327
293	31.7269	31.67
308	32.1294	31.984
400	35.86127	34.016 @ 387.3 (bp)

If the results of Haws and Harden, and those of Jhon, Grosh, and Eyring are compared with the properties tabulated in the N.A.S.A. Design Guide, the results of Haws and Harden are found to compare favorably with those listed in the Design Guide. For the purposes of the present study, then, the equations of Haws and Harden will be used to provide standards against which to compare the results of numerical computations made using the N.A.S.A. equilibrium composition analysis computer program. These computations are described in detail in subsequent sections of the present work. For the moment it is sufficient to note that in these computations each specie is assumed to be a perfect gas.

Of the major products of hydrazine decomposition, the only one which can liquify in the range of temperatures and pressures of present interest is ammonia. Since a gas is usually quite imperfect thermally near saturation its exact thermodynamic properties under these conditions are of considerable interest to one wishing to refine equilibrium composition calculations.

The thermodynamic properties of ammonia have been tabulated and graphically presented in the N.A.S.A. Design Guide (1966). Specific properties of interest, which are listed, are 1) the vapor pressure of liquid ammonia, and 2) the density of saturated ammonia vapor, 3) the density of liquid ammonia as a function of both pressure and temperature, 4) the heat capacities, and 5) the heat of vaporization.

The heat of formation of gaseous ammonia is -11.02 kcal/mole (Penner, 1968). Equations of state which may be used for ammonia are 1) the Berthelot equation, 2) van der Waals, 3) Beattie-Bridgeman, and 4) the Dieterici equation. The equations given below are taken from Penner (1968). The Berthelot equation is

$$V = \frac{RT}{p_c} + \frac{9RT_c}{128p_c}\left[1 - \frac{6T_c^2}{T^2}\right] \tag{15}$$

where p_c and T_c are respectively the critical pressure and temperature. The gas constant R for ammonia is obtainable, for any set of units, from the N.A.S.A. Design Guide.

The van der Waals equation would give

$$\left[p + \frac{a}{V^2}\right]\left[V - b\right] = RT \tag{16}$$

where $a = 3p_cV_c^2$ and $b = V_c/3$.

The Beattie=Bridgeman equation for gaseous ammonia is

$$p = RT\left[1 - \frac{c}{VT^3}\right]\frac{1}{V^2}\left[V + B_o - \frac{bB_o}{V}\right] - \frac{A_o}{V^2} - \frac{aA_o}{V^3} \tag{17}$$

where $A_o = 2.3930$

$B_o = 0.03415$

$a = 0.17031$

$b = 0.019112$

$c = 476.87 \times 10^{-4}$

for units in atmospheres, liters per mole, and °K.

The Dieterici equation, which is very accurate near critical points, is

$$\left[P e^{\frac{a}{VRT}} \right] (V - b) = RT \tag{18}$$

where $a = 7.39 p_c V_c^2$ and $b = V_c/2$.

The values for the constants in these equations are from Hirschfelder, Curtiss, and Bird (1954).

The remainder of this review is concerned with papers treating the decomposition of hydrazine.

K. W. Michel and H. Gg. Wagner (1965) studied the thermal decomposition of N_2H_4 diluted with argon and/or helium, behind shock waves, in the temperature range 1100 °K to 1600 °K, for pressures from 26.65 atm to 80.0 atm. For temperatures between 1100 °K and 1200 °K, decomposition did not start until an 'induction period' had passed. For temperatures greater than 1300 °K, the decomposition reaction begins by following a first-order reaction-rate law, and then changes to successive reactions of varying order.

A reaction of order one follows a rate law such as

$$-\frac{dc}{dt} = k_1 c \tag{19}$$

where c = specie concentration, k_1 = the rate constant, and t = time. Reactions may have an order greater than one. An example of such a reaction is

$$A + B \longrightarrow X + Y . \tag{20}$$

Let c_A be the concentration of specie A and c_B be the concentration of specie B. Let the superscript o indicate the value of a quantity at time t = 0. The reaction rate equations are

$$-\frac{dc_A}{dt} = -\frac{dc_B}{dt} = k_2 c_A c_B . \tag{21}$$

Define $x = c_A^o - c_A = c_B^o - c_B$

$$\frac{dx}{dt} = k_2 (c_A^o - x)(c_B^o - x) . \tag{22}$$

If, as a special case, $c_A^o = c_B^o$, then

$$\frac{dx}{dt} = k_2(c_A^o - x)^2 \tag{23}$$

$$-\frac{dc_A}{dt} = k_2 c_A^2 . \tag{24}$$

Many reactions are not as simple as those given above, and the reaction order may be non-integer in value.

The results of Michel and Wagner's investigation confirmed the "straight-chain" model for the decomposition reaction which had been proposed by G. K. Adams and G. W. Stock (1953). Reaction models for the hydrazine break-down are discussed later. At higher temperatures, the reaction rates were found to be partially dependent on the total gas density. For a density of 7.5 x 10^{-5} moles/cm^3, (26.65 atm),

$$\log k = 12.8 - ((52{,}000 \text{ cal/mole})/2.3RT) \tag{25}$$

and for a density of 2.5 x 10^{-5} moles/cm^3, (80.0 atm)

$$\log k = 12.0 - ((48{,}000 \text{ cal/mole})/2.3RT). \tag{26}$$

The main objective of the investigation was to determine the effects of small amounts of oxygen on the decomposition rate. It was found that small amounts (i.e. 0.2% of the mixture) do not affect the reaction. For temperatures above 1400 °K, heavy concentrations of oxygen, (e.g. $[O_2]/[N_2H_4] = .10$) still do not affect the decomposition reaction.

The amount of ammonia formed during the decomposition was also determined. It was found that at 1100 °K the ratio of NH_3 formed per amount of N_2H_4 decomposed is equal to one, at 1600 °K equal to 0.5, and at 2000 °K equal to zero. The radical NH appeared for temperatures above 1400 °K.

R. Roback (1965) made an investigation into the thermodynamic properties and equilibrium compositions of the products of dissociation of hydrogen, ammonia, and other materials, such as graphite, molybdenum, tungsten, and the carbides, nitrides, and oxides of titanium and zirconium. The temperature range was from 1800 °R (1000 °K) to 10,000 °R (5550 °K) for a pressure of 1000 atm. The materials considered were for use in controlling the radiation heat transfer to the moderator walls of gaseous nuclear-engined missles. The computations were carried out by assuming that all species obeyed the ideal gas law. Viscosities and thermal conductivities were obtained using data valid at one atm pressure, and a pressure correction determined from the Enskog theory for dense gases. Atomic and molecular species were considered in the computation, but ionic species were considered to be of negligible importance below a temperature of 10,000 °R (5550 °K). The calculations indicated that hydrogen dissociation is important for temperatures above 7000 °R (3880 °K). By contrast, concentrations of ammonia are almost completely decomposed into H_2 and N_2 at 2000 °R (1110 °K). Densities and enthalpies were computed for hydrogen, ammonia, and other gases, and presented as functions of temperature.

I. J. Eberstein and I. Glassman (1965) experimentally studied the decomposition of low concentrations of hydrazine for a temperature range of 750 °K to 1000 °K. The apparatus used was an adiabatic flow reactor with a driving pressure of 136 atm. Both the rate constants and reaction stoichiometry were determined. For hydrazine break-down inside a 3-inch duct, the reaction rate constant was determined to be

$$k = 10^{10.33} \exp(-36{,}170/RT) \ \mathrm{sec}^{-1}. \tag{27}$$

The over-all reaction, of an order close to one, was given as

$$N_2H_4 \longrightarrow 0.9NH_3 + 0.5N_2 + 0.6H_2 \, . \tag{28}$$

The stoichiometry of the reaction was determined by experiment.

Hydrazine-water mixture decomposition was also studied. For mixtures where the water was more then one percent of the total volume, the rate of decomposition was decreased by a factor of ten. The reaction rate for these mixtures was found to be independent of the amount of water present in the mixture, provided that the amount of water was more than one percent of the total volume. It was concluded that water must suppress one of the decomposition reaction steps.

Along with hydrazine, both unsymmetrical dimethyl hydrazine and monomethyl hydrazine were considered. Of the three, anhydrous hydrazine, N_2H_4, had the slowest decomposition rate.

E. J. Bair <u>et al</u>. (1966) used the explosive decomposition of hydrazine as part of their experimental program in the development of a high-resolution spectrometer and the spectroscopic procedures in examining explosive reactions. The reaction was described as a series of "free radical chain processes". One of the first products to be formed was NH_2, but this product dissappeared as the reaction continued, forming NH. The NH radical in turn also disappeared. Both radicals were observed spectrometrically. When the NH radical vanished, a spectrum of lines in the 0.600μ region was found which was thought to arise from the formation of N_2H_3, termed the "hydrazil radical".

A. S. Sokolik, V. P. Korpov, and E. S. Semenov (1967) used hydrazine decomposition flames in their study of turbulent burning rates and flame velocities. The decomposition process was considered to be a "straight-chain mechanism." The breaking of the reaction chain, however, is dependent on pressure. The reaction order is also dependent on reaction pressure. At low pressures, the order is approximatedly 1.0, and at high pressures the order is 1.5. It was noted that hydrazine "decomposes extremely readily," requiring special care in both the handling and experimental procedures.

R. F. Sawyer and I. Glassman (1967) have examined the reactions between hydrazine and nitrogen dioxide, nitric oxide, oxygen, and oxygen-nitric oxide, by using an adiabatic flow reactor. For each reaction, the investigators determined reaction rates, activation energies for the over-all reaction, and the reaction orders. Reacting with oxygen, hydrazine forms water and nitrogen according to the reaction

$$N_2H_4 + O_2 \longrightarrow 2H_2O + N_2 \tag{29}$$

For a total pressure of 1.0 atm and temperatures between 950 °K and 1010 °K, the hydrazine/oxygen reaction rate law is expressed as

$$\frac{d[N_2H_4]}{dt} = - k[N_2H_4] \tag{30}$$

with

$$k = 10^{9.91}\exp(-37,200/RT)\ \text{sec}^{-1} \tag{31}$$

and a reaction order of one. The activation energy was 37.2 kcal/mole.

The reaction rate is dependent on the concentration (to power one) and independent of the concentration of oxygen. Oxidation was shown to be possible whether or not the hydrazine was decomposed prior to the reaction. The production of water by the reaction was believed to be responsible for slowing the rate of decomposition.

D. I. Maclean and H. Gg. Wagner (1967) studied the decomposition-flame structure for both ammonia-oxygen and hydrazine vapor, determining experimentally temperature and specie-concentration profiles. The initial temperatures of the hydrazine vapor were between 70 °C and 90 °C, for pressures of 0.01842 atm and 0.0342 atm. It should be noted that the only initial substance in combustion was the pure hydrazine, with no other chemical species present. The reaction, after ignition, proceeds without aid of any oxidizers, and is exothermic. For the hydrazine-vapor flame, a maximum temperature of 1350 °K was found by means of a thermocouple. The investigators believed the temperature reading to be too low, as the adiabatic flame temperature should be near 1700 °K.

It was found by experiment that increasing the flame speed decreased the rate of decomposition of the first few millimeters above the burner. A major factor in the rate of decomposition is pressure. By doubling the pressure, nearly twenty mole percent of the hydrazine was broken down within the first millimeter above the burner.

The concentrations of H_2, N_2, and NH_3, which are the products of the reaction, and the rate of the reaction, are not affected by changes in the initial temperature of the hydrazine vapor. The maximum temperature is not affected by changes in pressure.

E. F. Logan and J. M. Marchello (1968) decomposed hydrazine by means of an alternating-current glow-discharge flow reactor. Using several flow rates and electric currents, light emmission spectra were measured from 0.300 µ to 0.600 µ. The most intense spectrum was produced by molecular nitrogen. However, atomic nitrogen spectra were not observed. Both atomic and molecular hydrogen were observed. The emmision bands for ammonia were not found. The radicals NH, NH_2, were found but OH was not. The gaseous hydrazine vapor pressure was 1.91×10^{-2} atm.

It was found that 65% of the hydrazine is decomposed very rapidly, with the rest of the reactant decomposing at a slower rate.

The decomposition of hydrazine has also been used in the study of the dissociation energy of the N-H and N-N bonds.

I. P. Fisher (1965a, b), with G. A. Heath, experimentally determined the value for the dissociation energy of the N-H bond. The value was found by electron-impact measurements, and by using the relation

$$D(H - N_2H_3) = A(N_2H_3^+) - I(N_2H_3) \tag{32}$$

where A is the appearance potential of $N_2H_3^+$, I is the ionization potential of N_2H_3, and D is the dissociation energy of the N-H bond. The values which were found were

$$A(N_2H_3^+) = 11.3 \pm 0.1 \text{ ev} \tag{33}$$

$$I(N_2H_3) = 7.88 \text{ ev} \tag{34}$$

$$D(H-N_2H_3) = 78.0 \text{ kcal/mole} . \tag{35}$$

Values for bond strengths, and heats of formation and ionization potentials of several chemical species resulting from hydrazine decomposition were also determined (Fisher, 1965b).

Another study of bond dissociation energies, for the N-N bond, was made by H. A. Olschewski, J. Troe, and H. Gg. Wagner (1966). It was shown that the decomposition activation energy must be measured for decomposition at high pressures. A shock tube of 70 mm diameter was constructed and used in their experimental program, with driving pressures up to 200 atm being applied.

For decomposition at high pressures, and densities greater than 5×10^{-4} moles/cm^3, the experimental results provided the temperature dependence of the reaction rates. The reaction rates were then used in determining the unimolecular decomposition activation energy, which was found to be 55 ± 2 kcal/mole. The reaction rate for decomposition at high pressures was determined to be

$$k = 10^{13.6} \exp(-55{,}000/RT) \text{ sec}^{-1}. \tag{36}$$

This rate constant is for the over-all reaction, and not to be confused with the dissociation energy of the N-H bond.

Two papers were found which discussed the decomposition of hydrazine by catalytic means.

A. S. Keston (1967) carried out a theoretical study of catalytic reactors designed for hydrazine decomposition.* Transient and steady-state models were developed for temperature and specie-concentration profiles within the reactor, as functions of time and position. Both thermal and catalytic-induced decomposition were considered, with the inclusion of the effects of heat and mass transfer between the free-flowing gas, and gas contained within the catalyst material. The results of the computations were compared with data from hydrazine-fueled engine experiments where the Shell 405 catalyst was used, with very good agreement between the theoretical and experimental results. These models provide an indirect means by which the decomposition of hydrazine and ammonia may be computed.

A summary of the results of the steady-state reaction calculations of Keston is given on the following page. The values are for an axial distance of 0.25 feet from the inlet end of the catalytic reactor.

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* Temperatures varied from 1000 °K to 1330 °K and pressures varied from 7.6 atm to 71 atm.

Table 4. Summary of steady-state reaction computations of Keston

P atm.	T °K	Mole Flow Rate lbm/ft^2-sec	Mole Fractions			Fractional NH$_3$dissoc.
			H_2	N_2	NH_3	
7.59	1000	1.51	0.55 (0.59)	0.31	0.14 (0.10)	0.62
14.8	1020 (1000)	1.52	0.57 (0.59)	0.32 (0.33)	0.10 (0.07)	0.71
32.6	1054 (1076)	3.12	0.55 (0.56)	0.31	0.14	0.64
66.2	1120	6.29	0.53 (0.51)	0.31 (0.32)	0.16 (0.17)	0.57
71.0	1054 (1076)	2.43	0.57 (0.54)	0.32	0.12 (0.15)	0.69

The numbers in (-) represent experimental data differing from the theoretical computations.

The mole fractions of H_2 and N_2 produced by the reaction are nearly independent of variations in pressure and temperature. The mole fraction of hydrogen produced varied between 0.53 and 0.57, and the mole fraction of nitrogen produced varied from 0.31 to 0.32. Ammonia mole-fractions varied between 0.10 and 0.16. It was found that in the reaction, mole-fractions of ammonia reached a maximum with respect to axial distance in the reactor (or equivalently, time), and then declined in value. Between 57% and 71% of the NH_3 produced in the reaction decomposes to nitrogen and hydrogen.

It may be noted that for the maximum mass flow rate, hydrogen production was at a maximum, as was the fractional NH_3 dissociation. However, the temperature of the reaction reached a maximum for lower mass-flow rates.

At either 14.8 atm or 71.0 atm, there was maximum output of hydrogen, chiefly due to the maximum dissociation of ammonia.

A second study of catalyst-induced hydrazine break-down was made by C. F. Sayer (1970) who also used the Shell 405 catalyst. The purpose of the study was to examine the chemical kinetics and mechanisms involved in the break-down of liquid hydrazine in the presence of the catalyst.

Using the Shell 405 catalyst, the break-down resulted in a gas mixture which was reported to be 99.4% N_2 and 0.6% N_2H_4.** The vanishing of the hydrogen was attributed to " the conversion of the hydrazine molecule into the nydrazinium ion." If a rhodium catalyst was used instead of the Shell 405 catalyst, then the resulting gas mixture was nearly 50% N_2 and 50% H_2. It may be noted that a main component of the Shell 405 catalyst is iridium. The reaction with the Shell 405 catalyst was expressed as

$$(37) \qquad 3N_2H_4 \longrightarrow N_2 + 4NH_3 \,.$$

For the rhodium catalyst, the reaction was written as

$$(38) \qquad 2N_2H_4 \longrightarrow N_2 + H_2 + 2NH_3 \,.$$

For the production of hydrogen from hydrazine, the rhodium catalyst is obviously to be preferred.

Two references attest to the volatility of hydrazine. G. P. Sutton (1963) noted that hydrazine may spontaneously ignite with either nitric acid or hydrogen peroxide. It was also noted that hydrazine vapor may form explosive mixtures with air.

Sutton very briefly discussed the reaction of hydrazine with catalysts. The products of the decomposition reaction, the exact composition of the product mixture, and the pressure will depend on the type of catalyst used.

If impurities are present in liquid hydrazine, or in contact with hydrazine vapor, then the hydrazine will readily decompose exothermically.

** The reaction was stopped when the total pressure in the experimental apparatus reached 1.025 atm.

E. J. Bowen and A. W. Birley (1951) found by experiment that for very low pressures, and temperatures of the order of 100 °C, that mixtures of hydrogen peroxide and hydrazine vapors may co-exist for a brief period of time without reaction. However, decomposition will then take place.

A comparison among the results for hydrazine decomposition shows fair agreement between the investigations of Michel and Wagner (1965), Eberstein and Glassman (1965), Sawyer and Glassman (1966), and Maclean and Wagner (1966). Without the presence of a catalyst, the stoichiometry of the decomposition reaction is generally

$$(39) \qquad N_2H_4 \longrightarrow NH_3 + \tfrac{1}{2}H_2 + \tfrac{1}{2}N_2 \ . \quad ^*$$

By inducing decomposition with a glow-discharge at a pressure of 1.91 x 10^{-2} atm, Logan and Marchello (1968) obtained a gas mixture consisting of 46% H_2, 28% N_2, and 19% NH_3 for 85% hydrazine break-down.

C. F. Sayer (1970) found that catalyst-induced reactions give results different from the previous investigations mentioned above. Using the Shell 405 catalyst, one mole of hydrazine results in the formation of 1.33 moles of ammonia. The final gas composition is however 99.4% N_2, and 0.6% N_2H_4. If a rhodium catalyst is used, one mole of hydrazine decomposes into one mole of ammonia, with a final gas composition of 50% N_2, and 50% H_2. The chemical reactions were stopped when total system pressures exceeded 1.0 atm.

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* Reaction pressures varied considerably. The pressures in the experiments were

Michel and Wagner	26.26 atm to 80.0 atm
Eberstein and Glassman	136 atm
Sawyer and Glassman	1 atm
Maclean and Wagner	0.0184 atm to 0.0342 atm

A. S. Keston (1967), by theoretical means, found that for elevated pressures, the results of decomposition of hydrazine are mostly H_2 and N_2. As an example, for a pressure of 7.6 atm, and a temperature of 1000 °K the gas mixture consisted of approximately 54% H_2. 31% N_2, and 15% NH_3. The maximum temperature was 1120 °K, and the maximum pressure was 71.0 atm.

For relatively low pressures, and temperatures of the order of 1000 °K, the present numerical investigation shows that the products of the decomposition reaction are almost entirely hydrogen and nitrogen, with twice as many moles of hydrogen being produced as nitrogen.

In comparing these results with those of previous investigations, the agreement is not unreasonable. In previous studies, for very low pressures, one mole of hydrazine decomposed to approximately one mole of ammonia, and a half-mole each of hydrogen and nitrogen. If a rhodium catalyst is used, the products of the reaction are equal mole numbers of hydrogen and nitrogen, with no ammonia left at the end of the reaction.

For elevated pressures (Keston, 1967), hydrogen is the major product (54%) with lesser amounts of nitrogen (31%) and ammonia (15%). It may be seen that as pressure increases, for temperatures in the neighborhood of 1000 °K, the ammonia production declines, and hydrogen and nitrogen are produced in amounts which appear to approach a ratio of two to one. The present computational prediction is that for pressures in the neighborhood of 7.6 atmospheres and temperatures of about 1000 °K, the mole-fractions of the decomposition products are 34% nitrogen and 66% hydrogen.

Several reaction mechanisms have been postulated for the break-down of hydrazine.

Michel and Wagner (1964) have noted that the first two reaction steps have been theoretically determined and experimentally verified. These steps are

(40) $$N_2H_4 \longrightarrow 2NH_2$$

(41) $$NH_2 + N_2H_4 \longrightarrow N_2H_3 + NH_3 .$$

For low temperatures, the next steps would then be

(42) $$N_2H_3 \longrightarrow H + HNNH$$

followed by

(43) $$H + N_2H_4 \longrightarrow NH_3 + NH_2$$

or

(44) $$H + N_2H_4 \longrightarrow H_2 + N_2H_3$$

(45) $$NH_2 + HNNH \longrightarrow NH_3 + N_2 + H$$

(46) $$2NH_2 \longrightarrow NH_3 + NH$$

(47) $$M + NH_2 + H \longrightarrow NH_3 + M .$$

At temperatures of 1600 °K, the step

(48) $$2NH_2 \longrightarrow HNNH + H_2$$

preceeds reaction (6). For temperatures in the neighborhood of 2000 °K, step (6) could be replaced by the reaction

(49) $$HNNH \longrightarrow NNH + H .$$

Eberstein and Glassman (1965) considered two possibile reaction mechanisms. The simple mechanism was similar to the postulated mechanism of Michel and Wagner, except for the last step. Michel and Wagner assumed the reaction

(50) $$NH_2 + HNNH \longrightarrow NH_3 + N_2 + H$$

whereas Eberstein and Glassman consider the reaction to be

(51) $$N_2H_3 + NH_2 \longrightarrow NH_3 + N_2 + H_2 .$$

The assumed mechanism includes branching reactions. By numerical techniques, the investigators found that the reaction has four parts. In the first part, the formation of free radicals takes place. The reaction steps which follow can be characterized by "steady-state" rate constants. The third part of the reaction was characterized by decreasing first-order rate constants. In the last part, the concentrations of free-radicals and the over-all reaction rate rapidly declined. When compared with experimentally-measured stoichiometry and reaction-rates, the reaction mechanism was found to be "in good quantitive agreement."

The reaction mechanism which was postulated is tabulated as follows.

Initiation:

(52) $$N_2H_4 + X \longrightarrow 2NH_2 + X .$$

Propagation:

(53) $N_2H_4 + NH_2 \longrightarrow NH_3 + N_2H_3$

(54) $N_2H_3 + X \longrightarrow N_2 + H_2 + H + X$

(55) $N_2H_4 + H \longrightarrow NH_3 + NH_2$.

Branching:

(56) $N_2H_3 + X \longrightarrow NH + NH_2 + X$

(57) $N_2H_4 + NH \longrightarrow NH_2 + N_2H_3$.

Termination:

(58) $NH_2 + N_2H_3 \longrightarrow NH_3 + N_2 + H_2$

(59) $N_2H_3 + N_2H_3 \longrightarrow 2NH_3 + N_2$

(60) $N_2H_3 + H \longrightarrow N_2 + 2H_2$

(61) $NH_2 + NH_2 \longrightarrow N_2H_4$.

Sawyer and Glassman (1966) have tabulated the assumed mechanisms for reactions of hydrazine with nitrogen dioxide, nitric oxide, and oxygen. In the reactions given, the authors assumed that branching occurs before propagation.

Sokolik, Korpov, and Semenov (1967) have noted that the "chain" mechanism of Adams and Stocks is usually accepted. The steps for this mechanism are

(62) $N_2H_4 \longrightarrow 2NH_2$.

Continuation: (propagation)

(63) $N_2H_4 + NH_2 \longrightarrow NH_3 + N_2H_3$

(64) $N_2H_3 \longrightarrow N_2 + H_2 + H$

(65) $H + N_2H_4 \longrightarrow NH_3 + NH_2$.

The chain breaking is dependent on the reaction pressure. For low pressures, the branching and termination steps are

(66) $$H + N_2H_3 \longrightarrow N_2 + 2H_2$$

(67) $$NH_2 + N_2H_3 \longrightarrow NH_3 + N_2 + H_2 .$$

For high pressure reactions, the branching and terminal steps are

(68) $$H + NH_2 + X \longrightarrow NH_3 + X$$

(69) $$H + H + X \longrightarrow H_2 + X .$$

Logan and Marchello (1968), discussing the glow-discharge break-down of hydrazine, gave the following reaction steps as the mechanism of electron-induced decomposition. The first step is caused by the electron interaction

(70) $$N_2H_4 + e^* \longrightarrow N_2H_4^* + e .$$

The (*) indicates an activation state. The authors' spectrometer measurements indicated that $N_2H_4^*$ breaks down in two simultaneous reactions.

(71) $$N_2H_4^* \longrightarrow N_2H_3 + H$$

(72) $$N_2H_4^* \longrightarrow NH_3 + NH$$

The reactions which then follow are

(73) $$H + N_2H_3, \longrightarrow H_2 + N_2H_2$$

(74) $$NH + N_2H_4 \longrightarrow NH_3 + N_2H_2 .$$

The diazene (or diimide) decomposes as

(75) $$N_2H_2 \longrightarrow N_2 + H_2 .$$

In all of the assumed reaction mechanisms, N_2H_4 always participates in a later reaction step, as well as in the initial step. There is disagreement as to the exact steps of the reaction after the initial and propagation reactions.

Sayer (1970) formulated a hydrazine break-down mechanism involving the use of catalysts, to explain the results of his experiments. It was postulated that hydrazine molecules adsorb on the catalyst surface, and react with other hydrazine molecules which are "in solution" to form two "cis-hydrogen" atoms. Additional products of this reaction are two molecules of ammonia, with cis-diimide adsorbed on the catalyst surface. Two adjacent molecules of diimide then react to form nitrogen and hydrazine. The nitrogen desorbs from the catalyst surface, and is replaced by another hydrazine molecule.

H. S. Maddix (1965) discussed the break-down of ammonia in his study of gaseous discharge phenomena. The ammonia decomposition was induced by an electrical discharge in a tube. The observed reaction was

$$(76) \qquad 2NH_3 \rightleftharpoons N_2 + 3H_2 .$$

As the amount of ammonia decreased, the nitrogen concentrations steadily increased. The hydrogen concentrations first rapidly increased, the decreased, and then increased again. The changes in the amount of hydrogen were due to chemical adsorption of the hydrogen with the tube walls.

A second discussion of the decomposition of ammonia was provided by Roback (1965). It was noted that above 2000 °R, ammonia is almost entirely dissociated, the products being H_2 and N_2. Above 4000 °R, H, NH, and NH_2 concentrations become appreciable. For temperatures above 7000 °R, N_2 begins to decompose to single atoms of nitrogen.

Michel and Wagner (1965) included a study of the pyrolysis of NH_3, which showed that ammonia decomposition is a first-order reaction. For temperatures between 2100 °K and 2900 °K, and with a 'carrier' gas of argon, the reaction rate was

$$(77) \qquad k = 10^{15.64} \exp[-(79.5 \pm 2.5 \text{ kcal/mole})/RT] \text{ cm}^3\text{/mole-sec} .$$

For temperatures greater than 1400 °K, NH radicals will be present in the decomposition-products mixture.

As has been shown, values of thermodynamic properties of hydrogen, nitrogen, ammonia, and hydrazine are readily available. The properties of hydrazine have been determined from both experimental studies and theoretical computations. Empirical equations for the properties of hydrazine have been presented, and equations of state for both gaseous hydrazine and ammonia have been listed.

In the foregoing, previous studies of hydrazine decomposition have been summarized and discussed. The studies have shown that in general one mole of hydrazine decomposes into one mole of ammonia, one-half mole of hydrogen, and one-half mole of nitrogen. The exact stoichiometry of the reactions depends on both the temperatures and pressure of the reaction. The use of a catalyst can lead to increased production of both hydrogen and nitrogen. However, if the incorrect catalyst is used, very little hydrogen will result from the hydrazine decomposition.

The results of the previous investigations and present numerical study have, where possible, been compared.

As has been shown, the decomposition mechanism is quite complex, and there is still disagreement among researchers studying the hydrazine breakdown as to the exact steps in the reaction. Several of the investigations have included studies of ammonia decomposition, and these have been summarized.

It is clear that the properties of hydrazine are not as well determined as one would wish. Although previous studies are not in exact agreement, there is qualitative agreement among them. Much more experimental work, however, will have to be performed to determine the exact kinetics of the decomposition reaction mechanism.

THE COMPUTATIONAL METHOD

The computer program used in the present calculation of hydrazine decomposition was written by S. Gordon and B. J. McBride (1971), and listed in N.A.S.A. SP-273. The program was designed to compute the equilibrium composition of reacting chemical mixtures for given thermodynamic states, i.e. specified (T,P), (H,P), (S,P), (T,V), (U,V), or (S,V), where:

T = temperature, °K

P = pressure, newton/meter^2

V = specific volume, meter^3/kg

H = enthalpy, joules

S = entropy, joules/°K

U = internal energy, joules.

The chemical species may be either in a gaseous phase and/or in a condensed phase.

The computer program also has the capability of computing rocket performance parameters, incident and reflected shock parameters, and Chapman-Jouguet detonation properties.

The method used for the present set of equilibrium composition calculations is based on the concept that reacting chemical systems are in equilibrium when the free-energy of the system is at an extremum value. The specified thermodynamic variables in this report are always pressure and temperature. The appropriate thermodynamic function for these variables is the Gibbs free energy function. As shown by J. B. Callen (1960), this function will possess a minimum. The minimization of the Gibbs free energy is constrained by additional physical conditions. For chemical reaction systems, one appropriate condition is that the mass involved in the reactions be conserved. When a given function possesses an extremum value, which is to be determined under one or more restraining conditions, the most suitable technique for determining this is the method of Lagrangian multipliers.

The alternative method of calculating chemical equilibrium composition is by using sets of simultaneous equilibrium equations in terms of equilibrium constants. The differences between the two methods, with their advantages and disadvantages, has been discussed by F. J. Zeleznik and S. Gordon (1960, 1966, 1968), and S. Gordon (1970). The investivations and results reported in the above-cited papers formed the basis for the computational method and program outlined by S. Gordon and B. J. McBride (1971).

Gordon (1960, 1970) has shown that if 'generalized' methods of solution are used to solve equilibrium problems expressed in either free-energy terms, or by equilibrium constant equations, the resulting sets of equations will reduce to the same number of equations to be solved. However, the 'constant' method has disadvantages not present in the free-energy method. The first of these, as noted by Gordon (1970), is "more bookkeeping". In using the 'constant' approach, the components (amounts) of the reactants and products must be selected, and the possible reactions written in terms of these components. Furthermore, equilibrium constants must be computed. It may be noted that such constants are not always available in the literature for high pressures and/or temperatures. The free-energy method does not require any part of the above-mentioned procedures.

If a chemical species is present in only trace amounts, i.e. "small components," then problems will occur in numerically solving the equilibrium constant equations. In the free-energy method, numerical difficulties are easily circumvented.

When one or more species is present in the form of a condensed phase (liquid and/or solid), the composition problem is very difficult to solve using the 'constant' approach, but is much easier to solve by the free-energy technique.

If non-ideal equations of state are to be used, then the 'constant' method will be very difficult to use, as the generalized solution methods are not very amenable to such modifications.

Partition functions may also be used in solving equilibrium problems. As shown by Lee, Sears, and Turcotte (1963), the equilibrium constant for a given chemical reaction may be expressed in terms of the partition functions of the reacting species. As an example, consider the reaction

$$X + Y = XY . \tag{1}$$

The equilibrium constant for the reaction is

$$K = \frac{Z_{XY}}{Z_X Z_Y} \tag{2}$$

where Z_X = the partition function for specie X

Z_Y = the partition function for specie Y

Z_{XY} = the partition function for specie XY .

The Gibbs free energy function can also be written in terms of the partition functions:

$$(3) \qquad G_f = -k'T \ln\left(\left[\frac{Z_X}{n_X^o}\right]^{n_X^o} \left[\frac{Z_Y}{n_Y^o}\right]^{n_Y^o} \left[\frac{Z_{XY}}{n_{XY}^o}\right]^{n_{XY}^o} \right)$$

where k'= the Boltzmann constant, and n_X^o, n_Y^o, and n_{XY}^o are the number of molecules of species X, Y, and XY at equilibrium.

Using the partition functions in the calculation of equilibrium chemical compositions involves computing equilibrium constants, a step which is not necessary in the free-energy method.

In the N.A.S.A. computer program, it is assumed that all gaseous chemical species will behave as ideal gases. For the high temperatures and pressures considered in the present work, the ideal gas law will be a fair approximation to the real behavior of the reacting system. The equation of state for ideal gases is written

$$(4) \qquad \frac{P}{\rho} = NRT$$

where $N = \sum_{j=1}^{m} n_j$

n_j = the number of kg-moles of the j^{th} species.

m = the number of species in the gas mixture

$n - m$ = the number of condensed species.

The following discussion is based in part on the material in the reports of Zeleznik and Gordon (1968) and Gordon and McBride (1971). The Gibbs free-energy function may be defined as

$$(5) \qquad G_f = G_f(T,P,n_j)$$

or equivalently,

$$(6) \qquad G_f = U - TS + PV$$

and as

(7)
$$dU = TdS - PdV + \sum_j^m \mu_j dn_j$$

then

(8)
$$dG_f = -SdT + VdP + \sum_j^m \mu_j dn_j$$

where the chemical potential (per kg-mole) is defined as

(9)
$$\mu_j = \left.\frac{\partial G_f}{\partial n_j}\right|_{T,P,\, n_k \neq j} .$$

The Gibbs function is homogeneous in n_j, i.e. the Gibbs function has the property that

(10)
$$G_f(T,P,\lambda n_j) = \lambda G_f(T,P,n_j) .$$

As previously mentioned, the Gibbs free energy function is appropriate in analyzing systems where the pressure and temperature are of constant value. It was also stated that the function will have a minimum value for a system in equilibrium. A system is considered to be in equilibrium if it is not changing, either mechanically, thermally, or chemically.

To show that the Gibbs function of a system is of minimum value when the system is in equilibrium, consider a system in contact with two 'reservoirs', one at constant temperature, the other at constant pressure. The general conditions for equilibrium are that

(11)
$$dU = 0$$

(12)
$$d^2U = 0 .$$

For an equilibrium situation, the total energy of the given system and the two 'reservoirs' must be of minimum value. Hence,

(13)
$$d(U + U_r) = 0$$

where r refers to 'reservoir' conditions. For the constant temperature reservoir,

(14)
$$dU_{r,T} = -T_r dS$$

and for the constant pressure reservoir,

(15) $$dU_{r,P} = P_r dV .$$

Therefore,

(16) $$d(U + U_r) = dU - T_r dS + P_r dV$$

(17) $$d(U + U_r) = d(U - T_r S + P_r V) .$$

Since the given system will have a temperature equal to T_r, and a pressure equal to P_r,

(18) $$d(U + U_r) = d(U - TS + PV)$$

(19) $$d(U + U_r) = dG_f$$

and the condition for equilibrium becomes, for constant temperatures and pressures,

(20) $$dG_f = 0 .$$

For chemically reacting systems, the equivalent condition is determined by using the Euler relation (Callen, 1960) and substituting into equation (18).

(21) $$U = TS - PV + \sum_{j=1}^{m} \mu_j n_j$$

The equilibrium condition then becomes

(22) $$d(\sum_{j=1}^{m} \mu_j n_j) = 0 .$$

To show that the condition is for a minmum value of the Gibbs function, consider the second derivative of the system energy.

(23) $$d^2(U + U_r) = d^2U + T_r d^2S + P_r d^2V = d^2G_f$$

and for the reservoirs,

(24) $$T_r d^2 S = 0$$

(25) $$P_r d^2 V = 0$$

and from equation (12),

(26) $$d^2(U + U_r) = d^2 G_f > 0 \,.$$

The Gibbs function thus has a minimum value for a system in equilibrium.

The free-energy per kilogram of gas mixture is, for constant temperature and pressure,

(27) $$g = \sum_{j=1}^{n} \mu_j n_j \,.$$

The condition for the mass balance of the reaction system needs to be considered. The expression for the mass balance is

(28) $$\sum_{j=1}^{n} a_{ij} b_j - b_i^o = 0 \qquad i = 1, \ldots, \ell$$

where a_{ij} = the stoichiometric coefficients (the kg-atoms of element i per kg-mole of specie j)

b_i^o = the specified number of kg-atoms of element i per kg of total reactants.

Define a function G as

(29) $$G = g + \sum_{i=1}^{\ell} \lambda_i (b_i - b_i^o)$$

where $b_i = \sum_{j=1}^{n} a_{ij} n_j$

λ_i = a Lagrangian multiplier

ℓ = the number of chemical elements.

Equation (29) represents the Gibbs Function, which is to be minimized, with the applied constraint. The condition for equilibrium becomes

$$(30) \qquad \delta G = 0 = \sum_{j=1}^{n} \left[\mu_j + \sum_{i=1}^{\ell} \lambda_i a_{ij} \right] \delta n_j + \sum_{i=1}^{\ell} (b_i - b_i^o) \delta \lambda_i \, .$$

If the variations in n_j and λ_i are independent, i.e. independent δn_j and $\delta \lambda_i$, then the resulting equilibrium equations are

$$(31) \qquad \mu_j + \sum_{i=1}^{\ell} \lambda_i a_{ij} = 0$$

$$(32) \qquad b_i - b_i^o = 0 \, .$$

It should be noted that λ contains the condition for phase equilibrium, and that the chemical potential of a species is the same for all phases of the species at a given temperature and pressure.

For the ideal gas equation of state, the chemical potential of the j^{th} species may be expressed as

$$(33) \qquad \mu_j = \mu_j^o + RT \, \ell n \left[\frac{n_j}{n} \right] + RT \, \ell n \, (P_{atm}) \qquad j = 1, \ldots, m$$

$$(34) \qquad \mu_j = \mu_j^o \qquad j = m + 1, \ldots, n$$

where μ_j^o is the chemical potential in the standard state, and P_{atm} is pressure given in terms of atmospheres.

The equations to be solved by Newton-Raphson iteration for the n_j, λ_i, and the numbers of moles, are listed in the report by Gordon and McBride. Details on initial estimates for the chemical composition, criteria for the covergence of the numerical solutions, tests for the possibility of condensed phases, and phase transitions, and mathematical singularities are also to be found in the report.

The thermodynamic data provided in the report with the program listing are mostly from the JANAF thermochemical property tables. For each chemical species, the specific heat for constant pressures, the enthalpy, and the entropy were computed from the following equations.

$$\frac{C_P^o}{R} = a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4 \tag{35}$$

$$\frac{H_T^o}{RT} = a_1 + \frac{a_2}{2}T + \frac{a_3}{3}T^2 + \frac{a_4}{4}T^3 + \frac{a_5}{5}T^4 + \frac{a_6}{T} \tag{36}$$

$$\frac{S_T^o}{R} = a_1 \ln T + a_2T + \frac{a_3}{2}T^2 + \frac{a_4}{3}T^3 + \frac{a_5}{4}T^4 + a_7 \tag{37}$$

where the a_k are 'least-squares' coefficients, which are provided in the program data deck. Two sets of coefficients are listed, for the temperature ranges 300 °K to 1000 °K, and from 1000 °K to 5000 °K. The use of either set of coefficients will give identical results at a temperature of 1000 °K.

DISCUSSION OF RESULTS

The results of the present set of computations for the decomposition of hydrazine are presented in both graphical and tabular form. The temperature range, from 300 °K to 1000°K, is divided into increments of 25 °K. The pressure range, from 1.0 atm to 610 atm, is divided into increments of 10 atm. The tabulated results are given in the appendix. The graphical presentation consists of three sets of figures, each set consisting of three figures, one for each of the reaction product species. The first set of figures are plots of mole-fraction (of H_2, N_2, or NH_3) vs temperature with pressure as the parameter. The second set of figures consists of graphs of mole-fraction vs pressure, with temperature as the parameter. The last set of figures consists of plots of temperature vs pressure with mole-fractions as the parameter.

For low temperatures and pressures, the decomposition products are approximately 2% H_2, 20% N_2, and 78% NH_3. For pressures greater than 50 atm, no H_2 is produced, and the product mixture is 20% N_2 and 80% NH_3. For higher temperatures (near 1000 °K) and low pressures, no NH_3 is left after the decomposition reaction has finished, and the product mixture consists of approximately 33% N_2 and 67% H_2. For high temperatures and pressures, the product mixture consists of approximately 59% H_2, 32% N_2, and 9% NH_3.

Trace amounts of NH and NH_2 may be found in the gaseous product mixture for elevated pressures and temperatures, but the amounts of these species are negligible.

It is clear that the effect of increasing the pressure, for a given temperature, is to decrease the amount of H_2 (and subsequently the amount of N_2) in the product mixture, and increase the amount of NH_3.

At low temperatures, the over-all decomposition reaction may be represented by

$$(1) \quad N_2H_4 \longrightarrow 1/3N_2 + 4/3NH_3 \ .$$

At higher temperatures, the over-all reaction may be represented by

$$(2) \quad N_2H_4 \longrightarrow N_2 + 2H_2 \ .$$

The low-temperature reaction (equation (1)) is in complete agreement with the results of the investigation made by C. F. Sayer (1970). For either case, the reaction is exothermic, and proceeds spontaneously. <u>Thus, any equilibrium calculation</u>, such as that given here, <u>will show no N_2H_4 concentration for any temperature</u>.

A comparison may be made between the results of the present computation and the results of A. S. Keston (1967). A summary of the results compared is given in the following table.

Table 5. Comparison of Keston results with present computations.

P, atm	T, °K	Mole Fraction (Keston)			Mole Fraction (present work)		
		H_2	N_2	NH_3	H_2	N_2	NH_3
7.59	1000	.55 (.59)	.31	.14	.665	.335	.0012
32.6	1054	.55 (.56)	.31	.14	.660	.330	.0059
71.0	1054	.57 (.54)	.32	.12 (.15)	.665	.328	.0110

The numbers in () indicate experimentally-determined values (Keston, 1967).

A comparison between the sets of results shows good agreement as to the amount of nitrogen produced. The discrepancies between the results are for the mole-fractions of hydrogen and ammonia. For both the theoretical predictions and experimental findings, Keston's results indicate that fewer moles of hydrogen will be produced, and many more moles of ammonia. Qualitatively, both investigations showed that an increase in the pressure for a given temperature will result in the production of more ammonia. It should be noted, however, that Keston's results are for steady flow of hydrazine across a Shell 405 catalyst bed. The data he presents do not appear to have reached zero rate of change with axial position in the catalyst bed and thus can be expected to show the lower H_2 concentrations than would equilibrium calculations; this is because most of the H_2 is produced by an endothermic decomposition of NH_3 which proceeds at a finite rate, evidently, slower than the transit time of the gas through the catalyst bed.

Two factors, in addition to the basic thermodynamic data used in the computation, certainly affect the accuracy of these results: The first is the condensation of one or more of the species at certain conditions and the second is the real gas behavior of the various species. One would expect that for the temperatures and pressures considered in the present investigation H_2 and N_2 behave substantially as perfect gases, far removed from saturation. NH_3, on the other hand, may easily saturate (see Table 6). Thus one should also consider the non-ideal nature of NH_3 for pressures and temperatures immediately above saturation in estimating the mole fraction of the various species present.

Table 6. Saturation curve of ammonia.

T ∿ °K	P ∿ atm
195.42 (T.P.)	0.05997
200	0.08553
210	0.1756
220	0.3347
230	0.5982
240	1.0124
250	1.6320
260	2.526
270	3.769
280	5.446
290	7.652
300	10.485
310	14.063
320	18.49
330	23.90
340	30.42
350	38.19
360	47.40
370	58.14
380	70.60
390	84.94
400	101.5
405.6 (C.P.)	111.5

Figure 10 compares the ideal NH_3 gas pressure for given density and temperature with the real gas pressure (Din, 1956) at the same conditions. The trends shown in the figure can be explained as follows: As the pressure increases at constant temperature the energy in the NH_3 molecule first tends to migrate from the translational degrees of freedom to the rotational or vibrational degree of freedom. Consequently the molecule transfers less momentum (exerts a smaller pressure) as the result of elastic collisions with other molecules than would be expected from a knowledge of its energy content. As one attempts to crowd more and more molecules of the same energy content into a given volume, collisions finally become so numerous that all the atoms in the molecule become involved more or less simultaneously, giving one the appearance of reducing the activity in the vibrational degree of freedom. This process is most apparent where the total energy content is small, e.g. at low temperatures, just above condensation. In the worst case the real gas pressure is about a factor of three lower than the ideal gas pressure for the same specific volume and temperature.

The results cannot be applied exactly to a mixture. The total pressure gives an indication of the crowding of the molecules but N_2 and H_2 molecules may induce a somewhat different response from NH_3 than NH_3 molecules on NH_3. Generally, one would expect that if the NH_3 in a mixture would suddenly go from a perfect gas to a real gas, the total pressure would drop somewhat (in proportion to the change in NH_3 pressure for the prevailing temperature and specific volume) and that the volume fractions of N_2 and H_2 would thereby increase somewhat. However, the total pressure is then somewhat lower and the NH_3 mole-fraction would then tend to increase. The net result is probably little different from that given by the perfect gas computations.

In comparing equilibrium computations with results for catalytic beds it is instructive to recall that an adiabatic catalyst can promote the redistribution of the energy brought to a reaction by the constituents but it does not add or withdraw energy (unless heated or cooled). In the case of hydrazine the initial reaction

$$3N_2H_4 \longrightarrow 4NH_3 + N_2 \tag{3}$$

is exothermic. If the energy released in this process is all used to effect the endothermic decomposition of NH_3 to N_2 and H_2 then when the temperatures and pressures of all the reaction products equals that of the incoming N_2H_4, the mole fractions of the product species will be as given by the equilibrium calculation. Viewed in this light the equilibrium calculations provide an upper bound for the effectiveness of a catalytic reactor.

In the real world, of course, things are not so simple. The reactor may have to be cooled, reducing the amount of heat available to decompose the NH_3. The reactions may not be complete when the constituents leave the reactive area and enter a region of lower pressure and lower temperature. In this region the reactions may freeze leaving the mole-fractions what they were leaving the reactive area or they may go to completion at the lower temperatures and pressures. In the latter case the NH_3 concentrations will be greater and the H_2 concentration lower than if the reactions froze. Thus to get large quantities of H_2 it is necessary to keep the reactants hot long enough for the NH_3 to decompose completely and then cool the mixture rapidly. Another factor to be considered in designing a reactor for H_2 production from N_2H_4 is the data of Sayer which indicated that a rhodium catalyst is more effective at promoting direct H_2 formation than the iridium (Shell 405) catalyst which seems to favor ammonia production as an intermediate step.

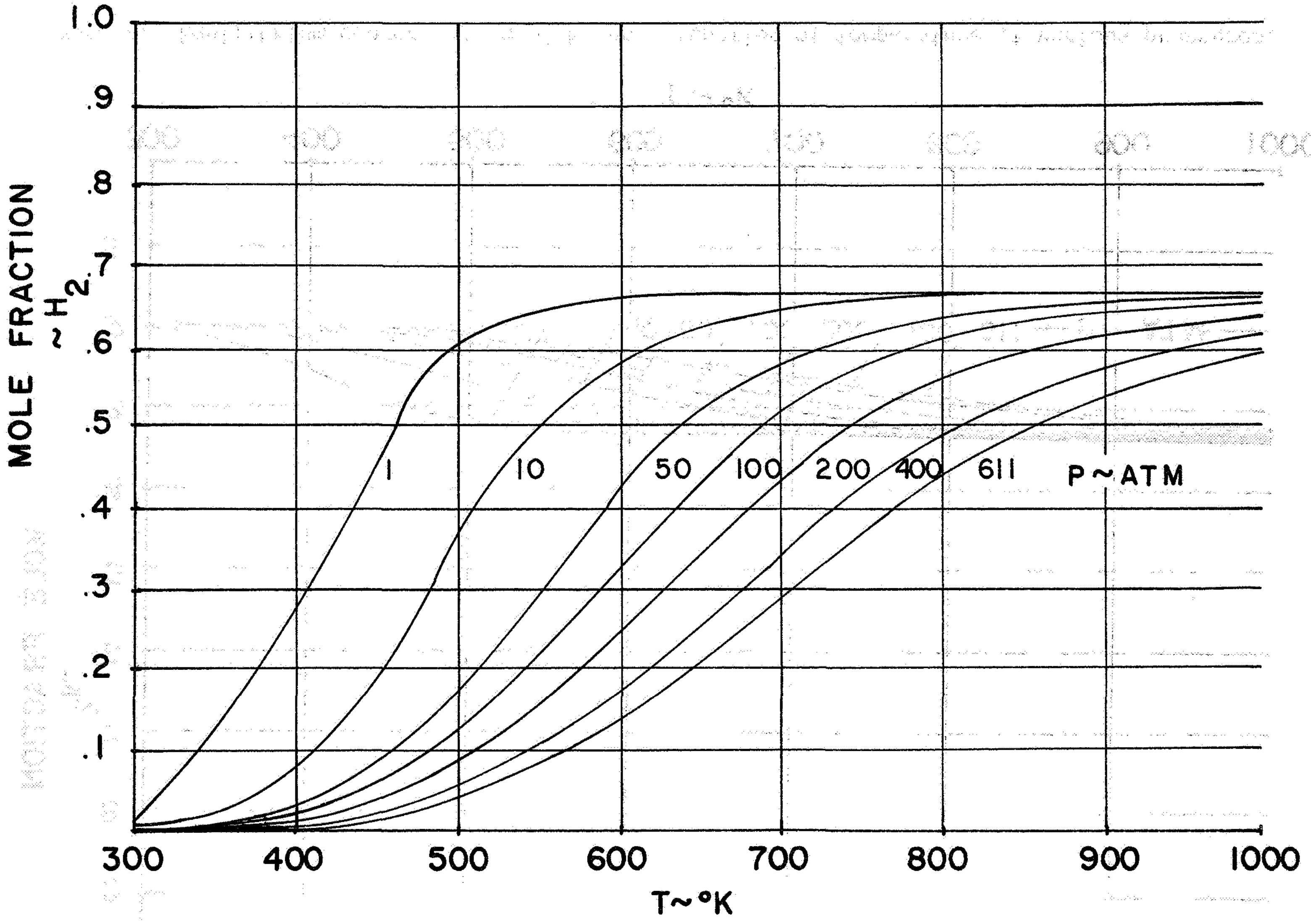


Figure 1. Equilibrium concentration of H_2 as a function of temperature at various pressures.

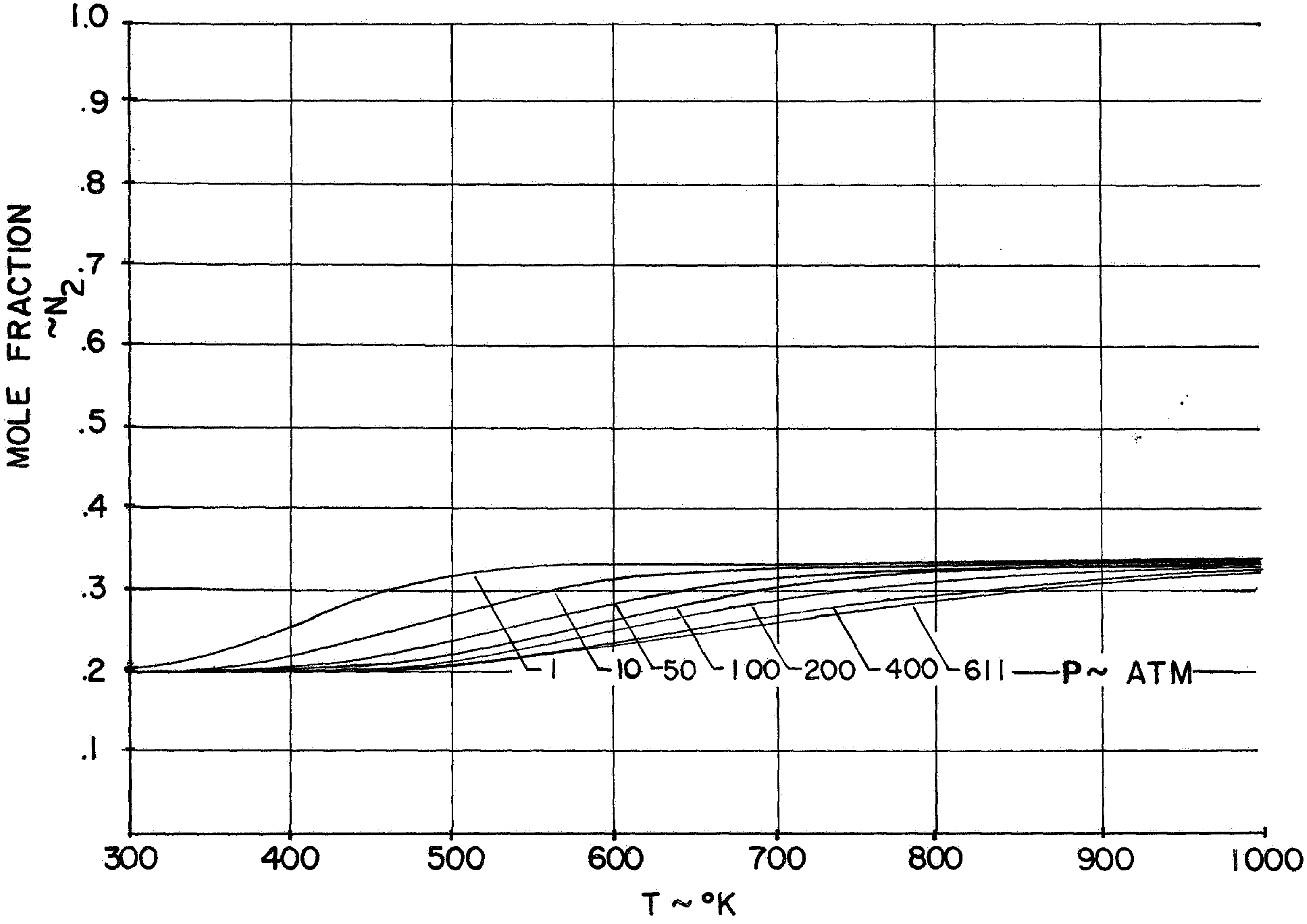


Figure 2. Equilibrium concentration of N_2 as a function of temperature at various pressures.

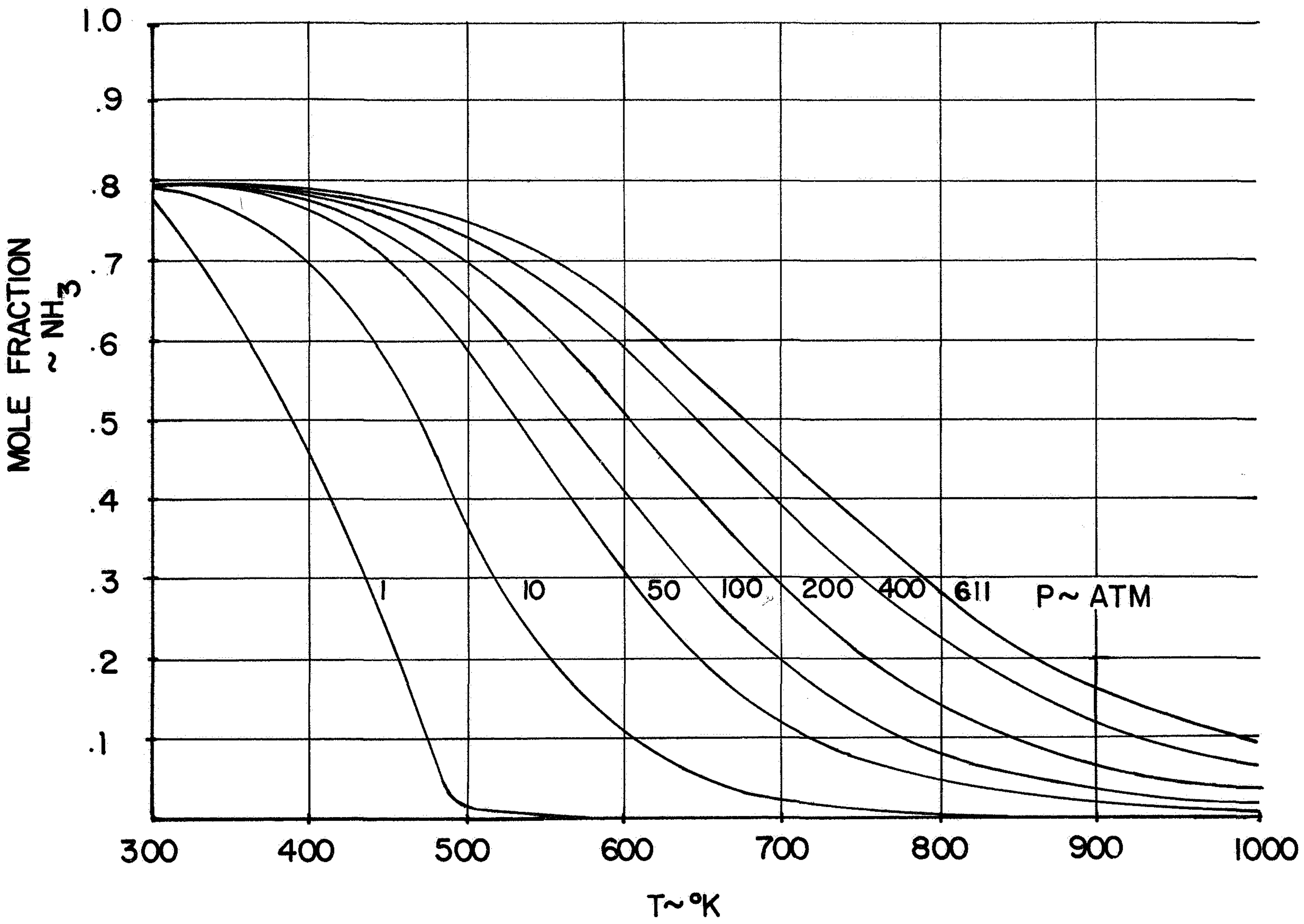


Figure 3. Equilibrium concentration of NH_3 as a function of temperature at various pressures.

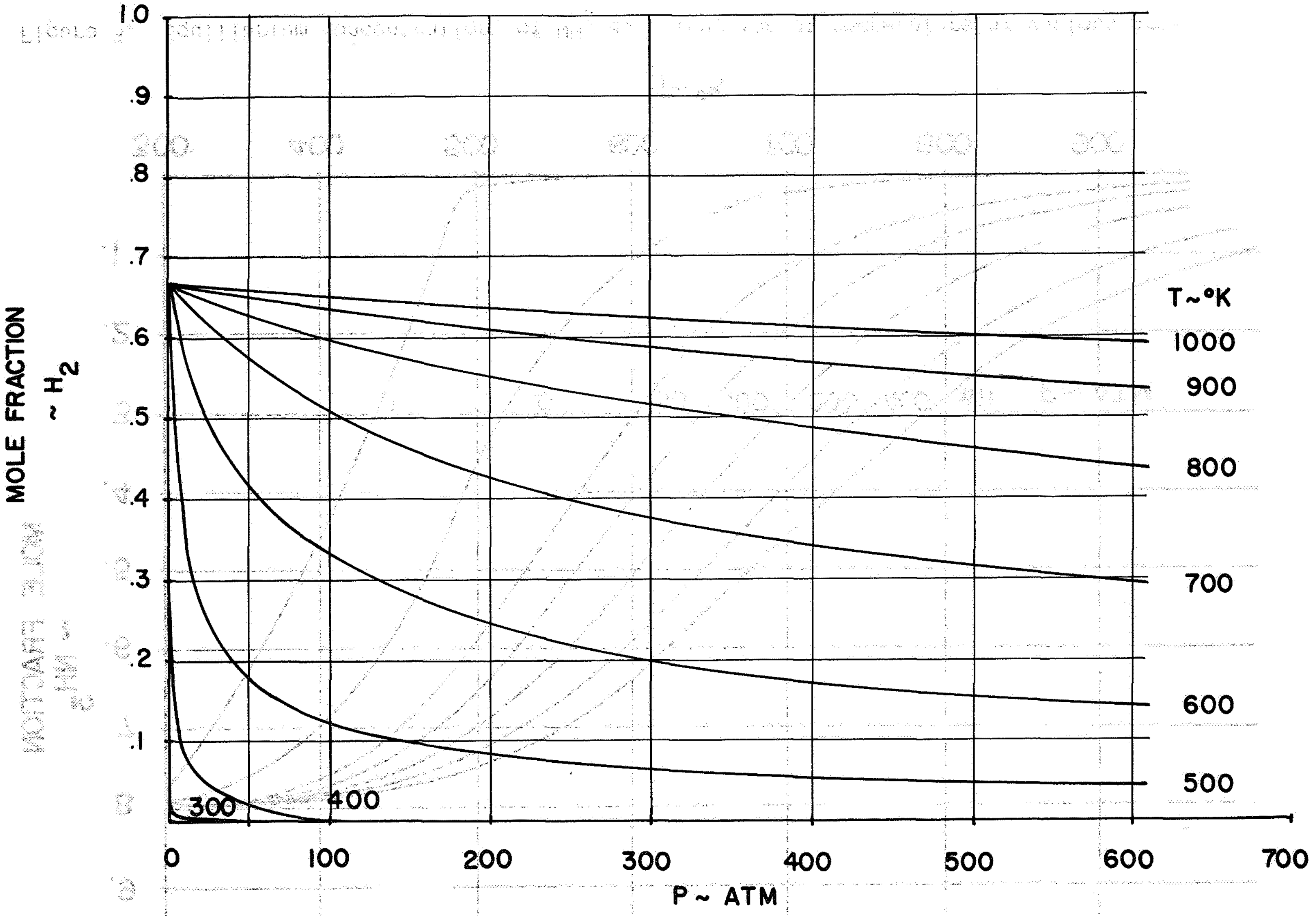


Figure 4. Equilibrium concentration of H_2 as a function of pressure at various temperatures.

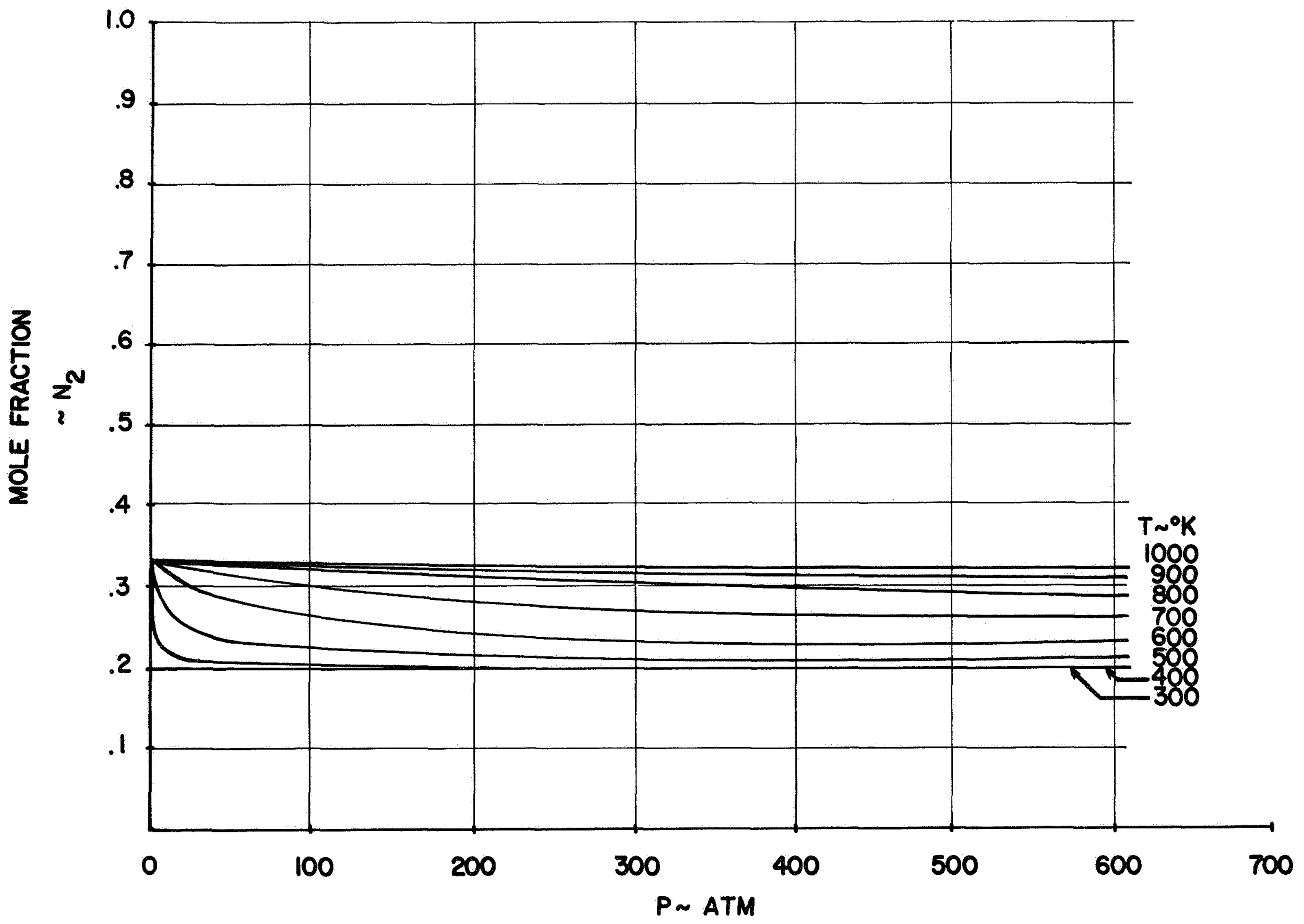


Figure 5. Equilibrium concentration of N_2 as a function of pressure at various temperatures.

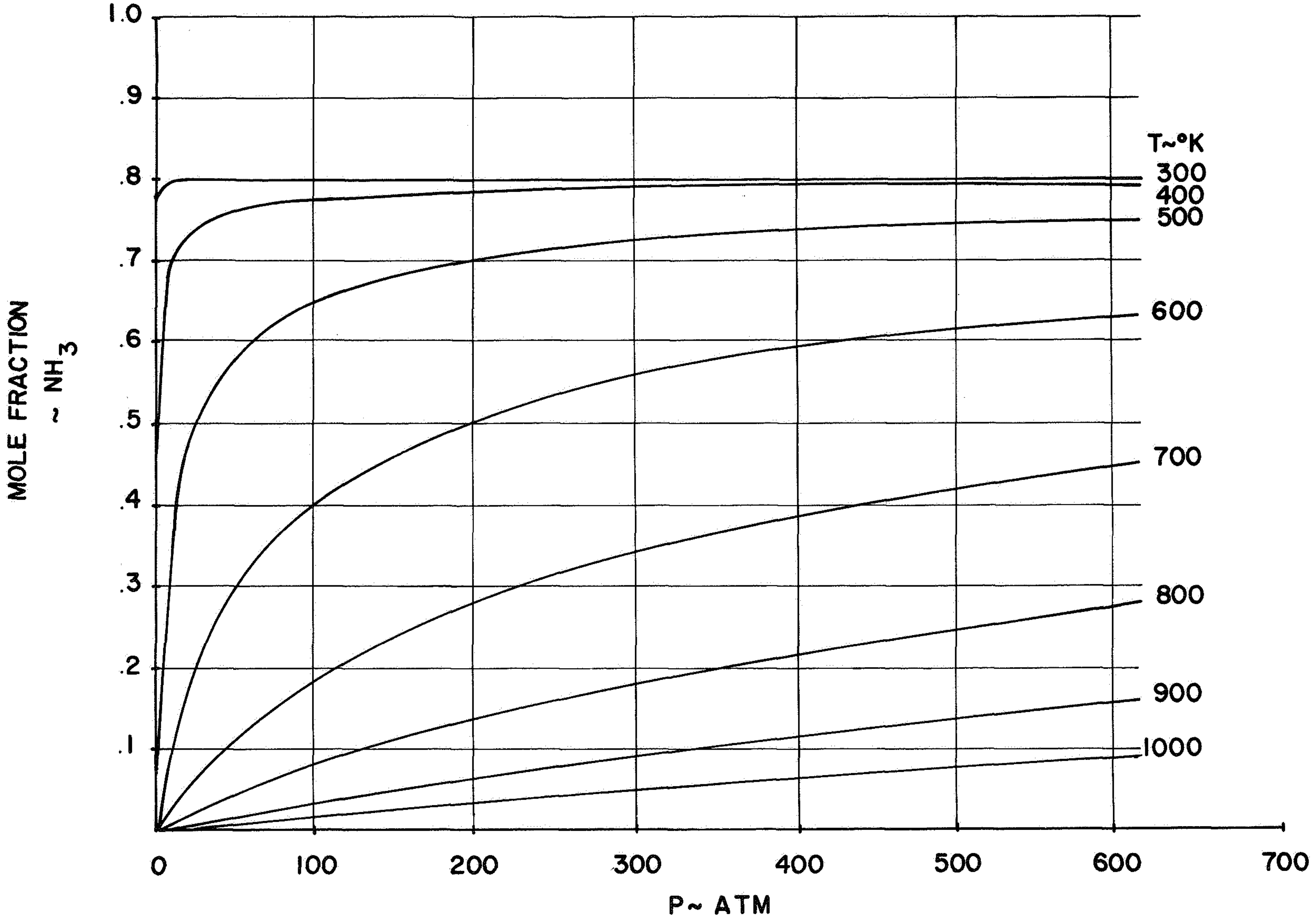


Figure 6. Equilibrium concentration of NH_3 as a function of pressure at various temperatures.

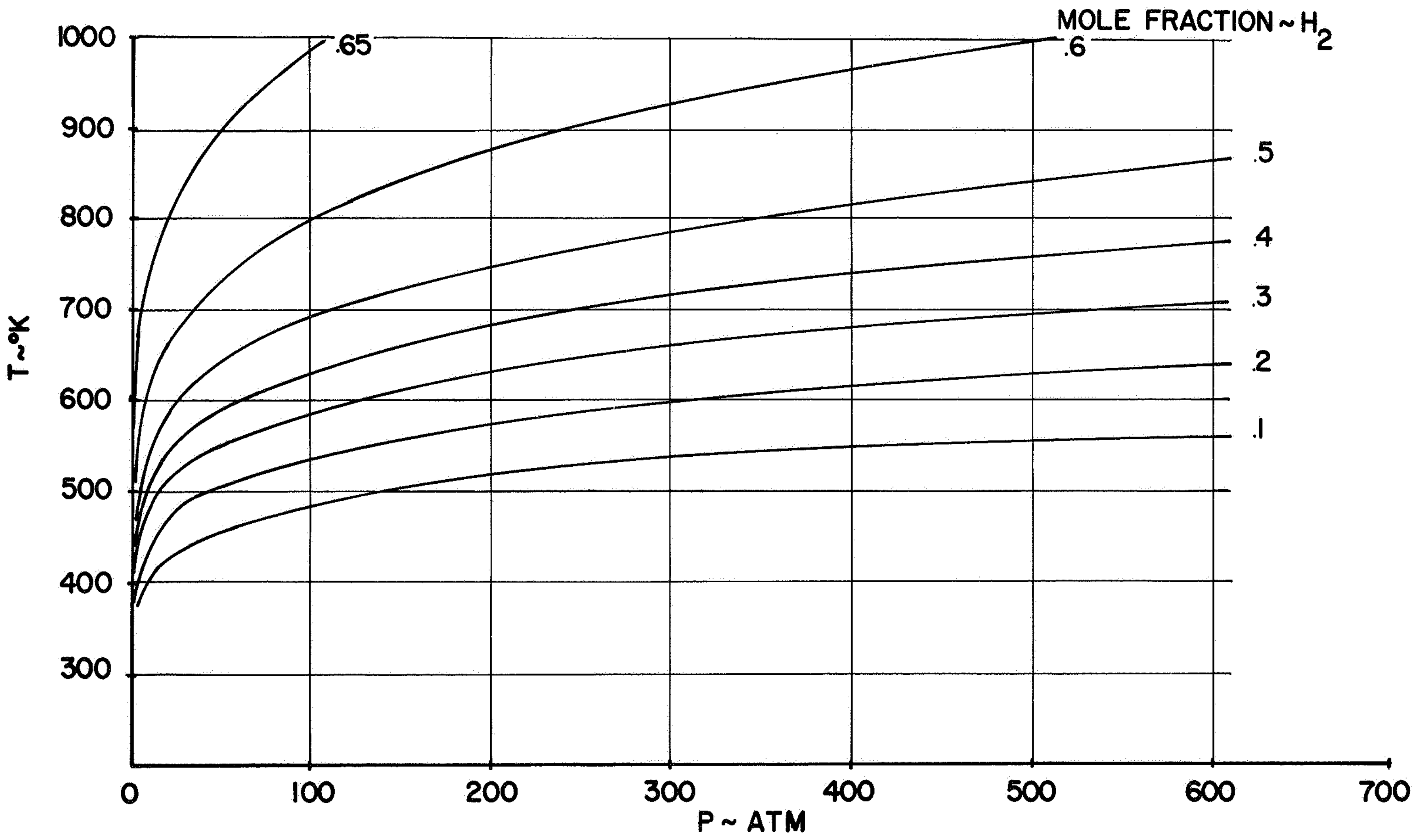


Figure 7. Variation of H_2 pressure with temperature for constant mole fractions.

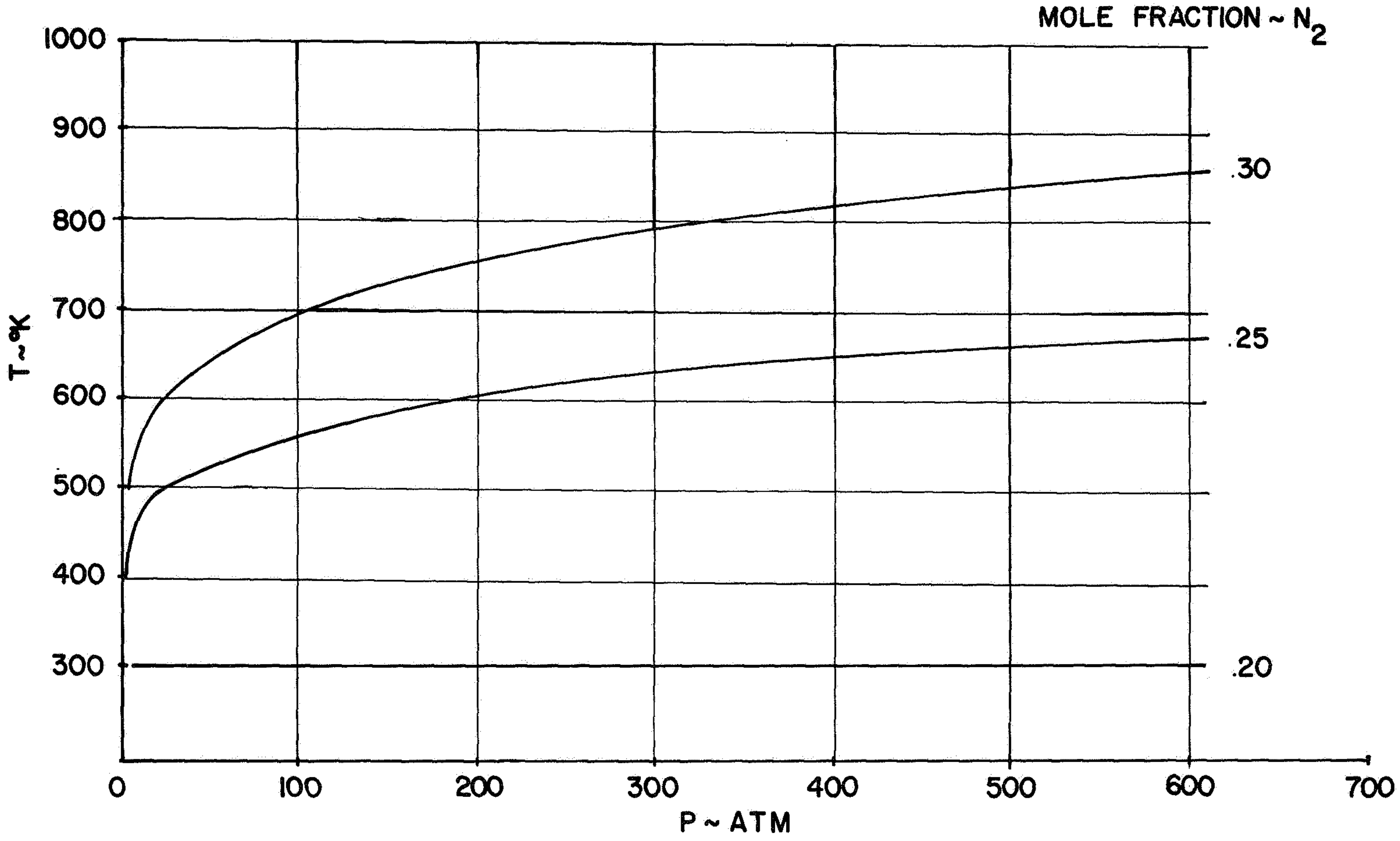


Figure 8. Variation of N_2 pressure with temperature for constant mole fractions.

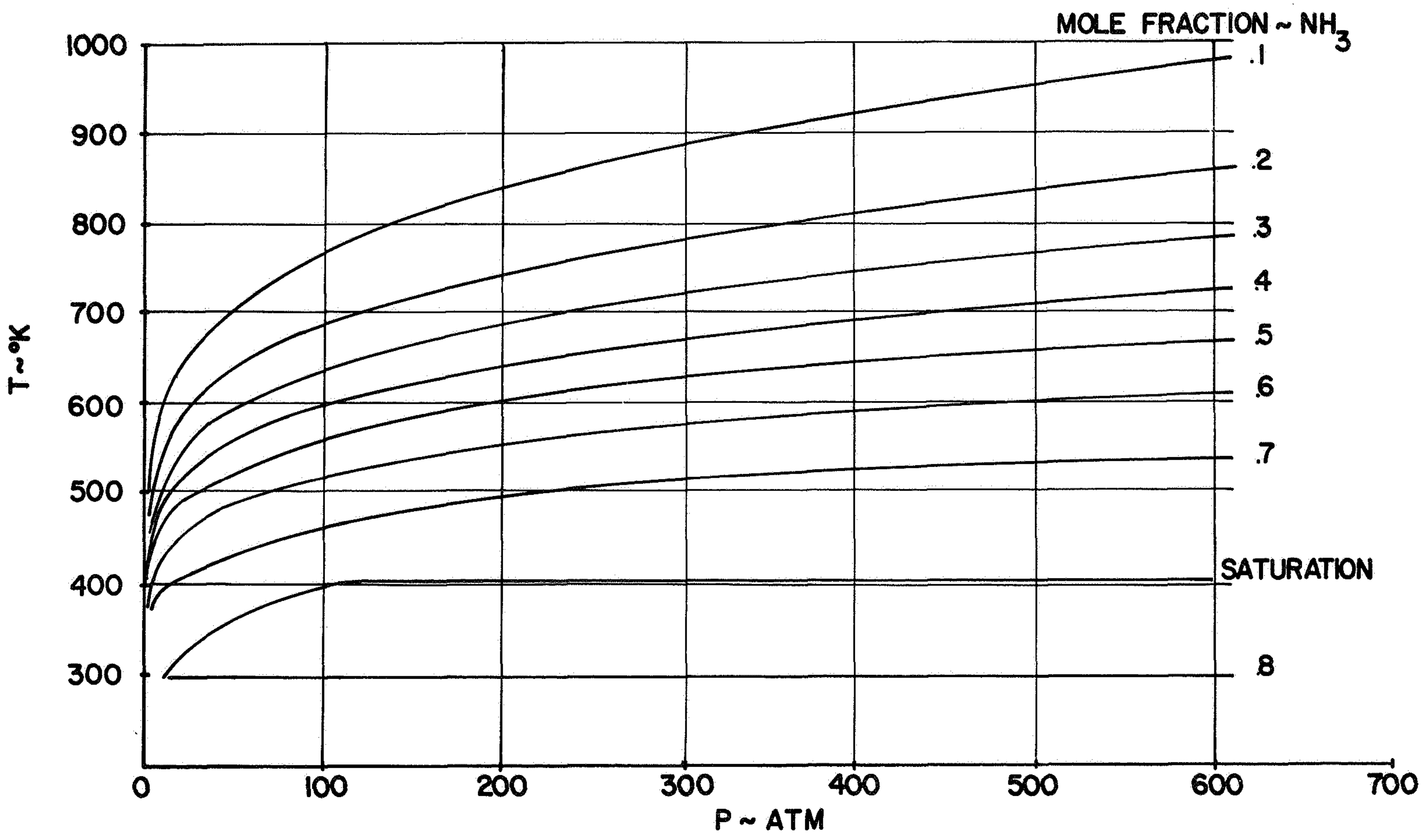
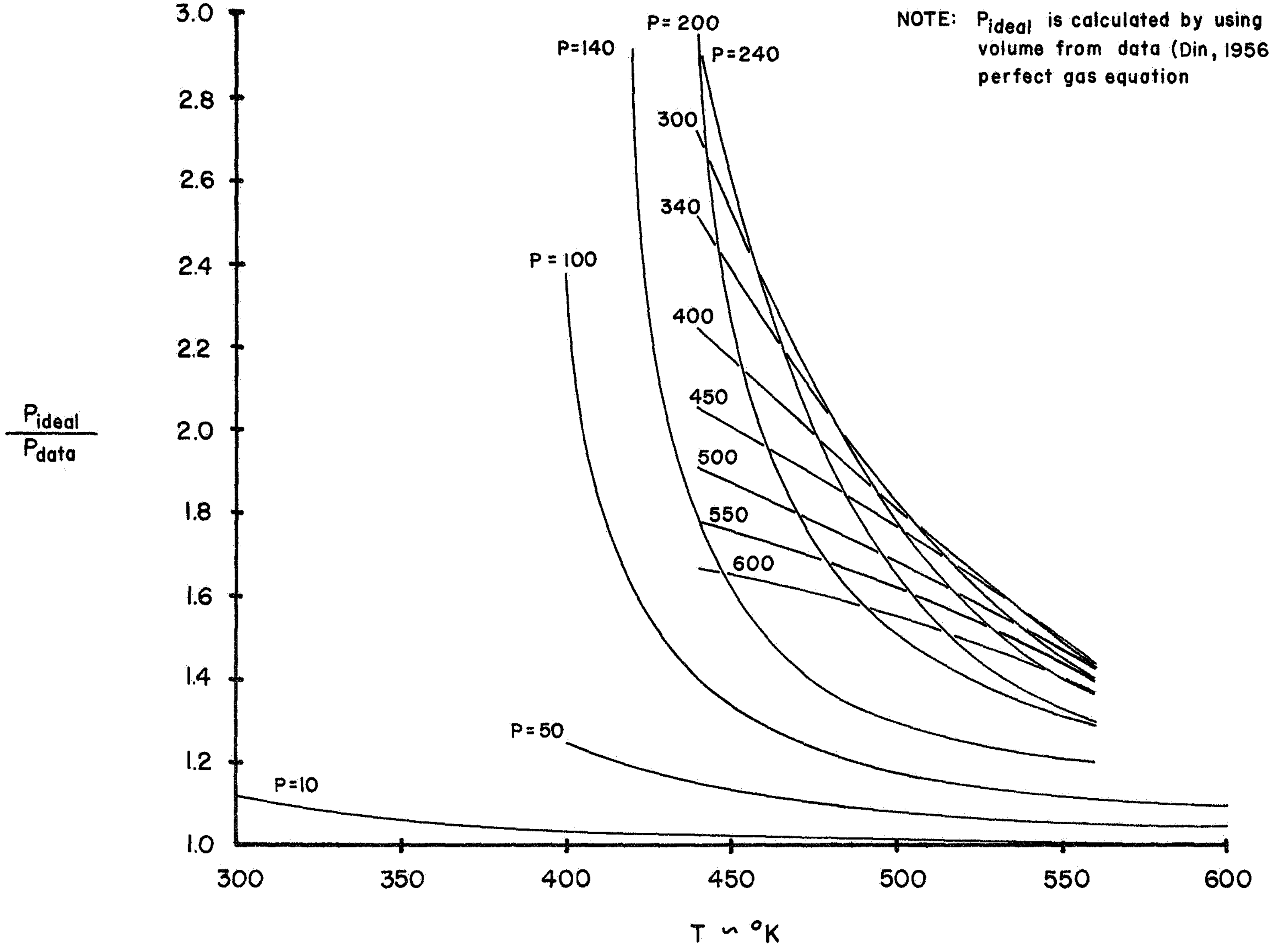


Figure 9. Variation of NH_3 pressure with temperature for constant mole fractions.



NOTE: P_{ideal} is calculated by using the specific volume from data (Din, 1956) in the perfect gas equation

Figure 10a. Comparison of the behavior of NH_3 with a perfect gas.

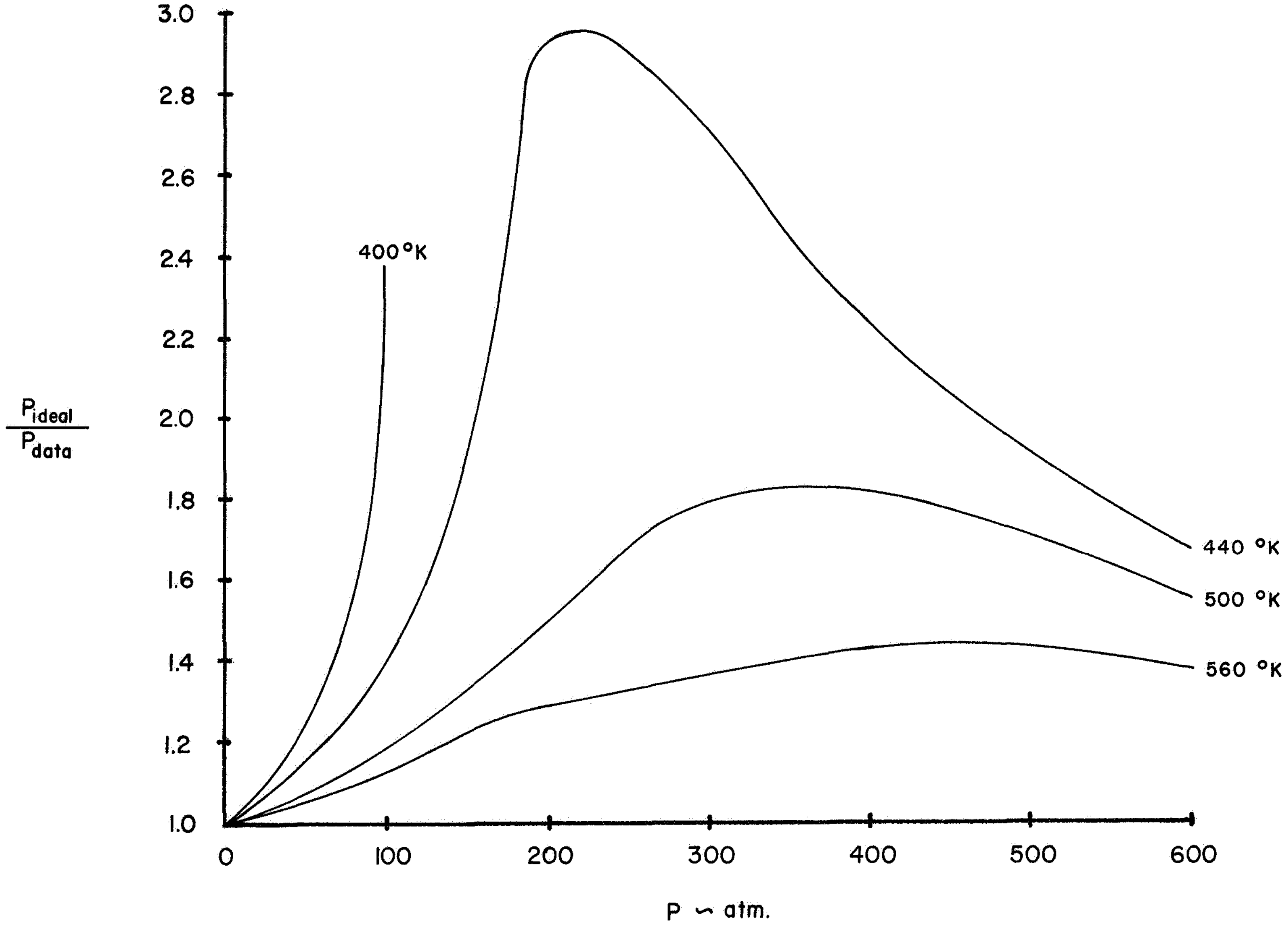


Figure 10b. Comparison of the behavior of NH_3 with a perfect gas.

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APPENDIX A - Nomenclature

A	Helmholtz free energy
a_{ij}	stoichiometric coefficient
b_i	$\sum_j a_{ij} n_j$
b_i^o	specified number of kg-atoms of element i per kg of total reactants
c_v	constant volume specific heat
c_p	constant pressure specific heat
G_f	Gibbs free energy function
g	Gibbs free energy per kg of gas mixture
H	enthalpy
K	equilibrium constant, general reaction equation
k	reaction rate constant
k'	Boltzmann constant
k_1	reaction rate constant for first order reaction
k_2	reaction rate constant for second order reaction
m	number of species in the gas mixture
N	total number of moles
n	number of species in the reacting system
n_X	number of moles of specie X
n_Y	number of moles of specie Y
n_{XY}	number of moles of reaction product XY
P	pressure
R	gas constant
S	entropy

T	temperature
t	time
U	internal energy
V	specific volume
Z	partition function
Z_X	partition function for specie X
Z_Y	partition function for specie Y
Z_{XY}	partition function for the reaction product XY
α	thermal expansion coefficient
β	compressibility
λ	Lagrangian multiplier
μ	chemical potential
ρ	density

Superscripts

o	quantity at equilibrium

Subscripts

c	value of quantity at the critical point
i	chemical specie indexing number
j	chemical specie indexing number
r	'reservoir' condition
T	value for specified temperature
$[O_2]$	brackets containing chemical symbols refer to concentrations of those chemical species.

Note: Duplicate symbols and/or other symbols appearing in the report are defined in the section where used.

APPENDIX B - Tabulation of Numerical Results

```
PRESSURE =    1.0 ATM.                 PRESSURE =   10.0 ATM.                 PRESSURE =   20.0 ATM.

TEMP    H2      NH3      N2            TEMP    H2      NH3      N2            TEMP    H2      NH3      N2
 300  0.0189  0.7773  0.2038            300  0.0042  0.7950  0.2008            300  0.0026  0.7968  0.2005
 325  0.0471  0.7434  0.2094            325  0.0107  0.7872  0.2021            325  0.0068  0.7919  0.2013
 350  0.0996  0.6804  0.2199            350  0.0239  0.7713  0.2048            350  0.0152  0.7817  0.2030
 375  0.1807  0.5831  0.2361            375  0.0476  0.7428  0.2095            375  0.0307  0.7631  0.2061
 400  0.2839  0.4593  0.2568            400  0.0855  0.6974  0.2171            400  0.0561  0.7326  0.2112
 425  0.3917  0.3299  0.2783            425  0.1393  0.6329  0.2279            425  0.0940  0.6872  0.2188
 450  0.4849  0.2181  0.2970            450  0.2076  0.5509  0.2415            450  0.1450  0.6260  0.2290
 475  0.5533  0.1360  0.3107            475  0.2851  0.4578  0.2570            475  0.2075  0.5510  0.2415
 500  0.5978  0.0827  0.3196            500  0.3641  0.3631  0.2728            500  0.2774  0.4672  0.2555
 525  0.6248  0.0502  0.3250            525  0.4368  0.2759  0.2873            525  0.3488  0.3815  0.2697
 550  0.6408  0.0310  0.3282            550  0.4978  0.2026  0.2996            550  0.4159  0.3009  0.2832
 575  0.6503  0.0196  0.3301            575  0.5454  0.1456  0.3091            575  0.4744  0.2307  0.2949
 600  0.6561  0.0127  0.3312            600  0.5805  0.1034  0.3161            600  0.5223  0.1733  0.3044
 625  0.6596  0.0085  0.3319            625  0.6054  0.0735  0.3211            625  0.5595  0.1286  0.3119
 650  0.6618  0.0058  0.3324            650  0.6229  0.0525  0.3246            650  0.5874  0.0951  0.3175
 675  0.6633  0.0041  0.3326            675  0.6351  0.0379  0.3270            675  0.6079  0.0705  0.3216
 700  0.6642  0.0029  0.3328            700  0.6435  0.0278  0.3287            700  0.6229  0.0526  0.3246
 725  0.6649  0.0021  0.3330            725  0.6495  0.0206  0.3299            725  0.6337  0.0396  0.3267
 750  0.6653  0.0016  0.3331            750  0.6537  0.0156  0.3307            750  0.6415  0.0301  0.3283
 775  0.6656  0.0012  0.3331            775  0.6567  0.0119  0.3313            775  0.6473  0.0232  0.3295
 800  0.6659  0.0009  0.3332            800  0.6590  0.0092  0.3318            800  0.6516  0.0181  0.3303
 825  0.6660  0.0007  0.3332            825  0.6606  0.0073  0.3321            825  0.6547  0.0143  0.3309
 850  0.6662  0.0006  0.3332            850  0.6618  0.0058  0.3324            850  0.6571  0.0114  0.3314
 875  0.6663  0.0005  0.3333            875  0.6628  0.0046  0.3326            875  0.6590  0.0092  0.3318
 900  0.6663  0.0004  0.3333            900  0.6635  0.0038  0.3327            900  0.6604  0.0075  0.3321
 925  0.6664  0.0003  0.3333            925  0.6641  0.0031  0.3328            925  0.6615  0.0062  0.3323
 950  0.6664  0.0003  0.3333            950  0.6645  0.0026  0.3329            950  0.6624  0.0051  0.3325
 975  0.6665  0.0002  0.3333            975  0.6649  0.0022  0.3330            975  0.6631  0.0043  0.3326
1000  0.6665  0.0002  0.3333           1000  0.6651  0.0018  0.3330           1000  0.6636  0.0036  0.3327
```

```
PRESSURE =   30.0 ATM.               PRESSURE =   40.0 ATM.               PRESSURE =   50.0 ATM.

TEMP    H2      NH3       N2         TEMP    H2      NH3       N2         TEMP    H2      NH3       N2
 300  0.0020  0.7976  0.2004          300  0.0017  0.7980  0.2003          300  0.0014  0.7983  0.2003
 325  0.0052  0.7938  0.2010          325  0.0043  0.7949  0.2008          325  0.0037  0.7956  0.2007
 350  0.0117  0.7860  0.2023          350  0.0097  0.7884  0.2019          350  0.0083  0.7900  0.2017
 375  0.0237  0.7716  0.2047          375  0.0196  0.7764  0.2039          375  0.0170  0.7796  0.2034
 400  0.0436  0.7477  0.2087          400  0.0364  0.7564  0.2073          400  0.0315  0.7621  0.2063
 425  0.0738  0.7114  0.2148          425  0.0620  0.7256  0.2124          425  0.0540  0.7352  0.2108
 450  0.1157  0.6611  0.2231          450  0.0981  0.6823  0.2196          450  0.0860  0.6968  0.2172
 475  0.1689  0.5973  0.2338          475  0.1449  0.6261  0.2290          475  0.1281  0.6462  0.2256
 500  0.2310  0.5228  0.2462          500  0.2010  0.5588  0.2402          500  0.1795  0.5845  0.2359
 525  0.2977  0.4427  0.2595          525  0.2632  0.4841  0.2526          525  0.2379  0.5146  0.2476
 550  0.3642  0.3630  0.2728          550  0.3274  0.4071  0.2655          550  0.2995  0.4405  0.2599
 575  0.4257  0.2892  0.2851          575  0.3893  0.3329  0.2778          575  0.3606  0.3672  0.2721
 600  0.4791  0.2251  0.2958          600  0.4452  0.2658  0.2890          600  0.4176  0.2989  0.2835
 625  0.5230  0.1723  0.3046          625  0.4931  0.2083  0.2986          625  0.4679  0.2386  0.2936
 650  0.5577  0.1307  0.3115          650  0.5323  0.1612  0.3065          650  0.5102  0.1877  0.3020
 675  0.5843  0.0988  0.3169          675  0.5634  0.1239  0.3127          675  0.5447  0.1464  0.3089
 700  0.6043  0.0749  0.3208          700  0.5873  0.0952  0.3175          700  0.5719  0.1138  0.3144
 725  0.6191  0.0571  0.3238          725  0.6056  0.0733  0.3211          725  0.5930  0.0884  0.3186
 750  0.6301  0.0438  0.3260          750  0.6193  0.0568  0.3239          750  0.6091  0.0690  0.3218
 775  0.6383  0.0340  0.3277          775  0.6297  0.0443  0.3259          775  0.6215  0.0542  0.3243
 800  0.6444  0.0267  0.3289          800  0.6376  0.0349  0.3275          800  0.6309  0.0429  0.3262
 825  0.6491  0.0211  0.3298          825  0.6435  0.0278  0.3287          825  0.6381  0.0342  0.3276
 850  0.6526  0.0169  0.3305          850  0.6481  0.0223  0.3296          850  0.6437  0.0275  0.3287
 875  0.6553  0.0137  0.3310          875  0.6516  0.0181  0.3303          875  0.6480  0.0224  0.3296
 900  0.6573  0.0112  0.3315          900  0.6543  0.0148  0.3309          900  0.6514  0.0183  0.3303
 925  0.6590  0.0092  0.3318          925  0.6565  0.0122  0.3313          925  0.6540  0.0152  0.3308
 950  0.6603  0.0077  0.3320          950  0.6582  0.0102  0.3316          950  0.6561  0.0126  0.3312
 975  0.6613  0.0064  0.3323          975  0.6595  0.0085  0.3319          975  0.6578  0.0106  0.3316
1000  0.6621  0.0054  0.3324         1000  0.6606  0.0072  0.3321         1000  0.6592  0.0090  0.3318
```

```
PRESSURE =   60.0 ATM.               PRESSURE =   70.0 ATM.               PRESSURE =   80.0 ATM.

TEMP    H2      NH3      N2          TEMP    H2      NH3      N2          TEMP    H2      NH3      N2
 300  0.0013  0.7985  0.2002          300  0.0011  0.7986  0.2002          300  0.0010  0.7987  0.2002
 325  0.0033  0.7961  0.2006          325  0.0029  0.7965  0.2006          325  0.0027  0.7968  0.2005
 350  0.0074  0.7911  0.2015          350  0.0067  0.7920  0.2013          350  0.0061  0.7926  0.2012
 375  0.0151  0.7819  0.2030          375  0.0136  0.7836  0.2027          375  0.0125  0.7850  0.2025
 400  0.0281  0.7663  0.2056          400  0.0254  0.7695  0.2051          400  0.0233  0.7720  0.2047
 425  0.0482  0.7421  0.2096          425  0.0438  0.7474  0.2088          425  0.0403  0.7517  0.2080
 450  0.0772  0.7074  0.2154          450  0.0703  0.7156  0.2141          450  0.0648  0.7222  0.2130
 475  0.1157  0.6612  0.2231          475  0.1059  0.6729  0.2212          475  0.0980  0.6824  0.2196
 500  0.1633  0.6041  0.2327          500  0.1504  0.6195  0.2301          500  0.1399  0.6321  0.2280
 525  0.2182  0.5382  0.2436          525  0.2024  0.5572  0.2405          525  0.1893  0.5729  0.2379
 550  0.2774  0.4671  0.2555          550  0.2593  0.4889  0.2518          550  0.2440  0.5071  0.2488
 575  0.3373  0.3952  0.2675          575  0.3178  0.4186  0.2636          575  0.3012  0.4386  0.2602
 600  0.3945  0.3266  0.2789          600  0.3747  0.3503  0.2749          600  0.3576  0.3709  0.2715
 625  0.4462  0.2646  0.2892          625  0.4272  0.2873  0.2854          625  0.4105  0.3074  0.2821
 650  0.4908  0.2111  0.2981          650  0.4734  0.2319  0.2947          650  0.4577  0.2507  0.2915
 675  0.5278  0.1667  0.3056          675  0.5124  0.1851  0.3025          675  0.4984  0.2019  0.2997
 700  0.5576  0.1308  0.3115          700  0.5445  0.1466  0.3089          700  0.5322  0.1613  0.3064
 725  0.5812  0.1026  0.3162          725  0.5701  0.1159  0.3140          725  0.5597  0.1284  0.3119
 750  0.5995  0.0806  0.3199          750  0.5903  0.0916  0.3181          750  0.5816  0.1021  0.3163
 775  0.6136  0.0636  0.3227          775  0.6061  0.0727  0.3212          775  0.5988  0.0814  0.3198
 800  0.6245  0.0506  0.3249          800  0.6183  0.0580  0.3237          800  0.6123  0.0652  0.3225
 825  0.6329  0.0405  0.3266          825  0.6278  0.0466  0.3256          825  0.6229  0.0525  0.3246
 850  0.6394  0.0327  0.3279          850  0.6352  0.0377  0.3270          850  0.6311  0.0426  0.3262
 875  0.6445  0.0266  0.3289          875  0.6410  0.0308  0.3282          875  0.6376  0.0348  0.3275
 900  0.6485  0.0218  0.3297          900  0.6456  0.0253  0.3291          900  0.6427  0.0287  0.3285
 925  0.6516  0.0181  0.3303          925  0.6492  0.0210  0.3298          925  0.6468  0.0238  0.3294
 950  0.6541  0.0151  0.3308          950  0.6521  0.0175  0.3304          950  0.6501  0.0199  0.3300
 975  0.6561  0.0127  0.3312          975  0.6544  0.0147  0.3309          975  0.6527  0.0168  0.3305
1000  0.6577  0.0108  0.3315         1000  0.6562  0.0125  0.3312         1000  0.6548  0.0142  0.3310
```

```
PRESSURE =   90.0 ATM.              PRESSURE =  100.0 ATM.              PRESSURE =  110.0 ATM.

TEMP    H2      NH3     N2          TEMP    H2      NH3     N2          TEMP    H2      NH3     N2
 300  0.0010  0.7988  0.2002         300  0.0009  0.7989  0.2002         300  0.0008  0.7990  0.2002
 325  0.0025  0.7970  0.2005         325  0.0023  0.7972  0.2005         325  0.0022  0.7974  0.2004
 350  0.0057  0.7932  0.2011         350  0.0053  0.7937  0.2011         350  0.0050  0.7940  0.2010
 375  0.0116  0.7861  0.2023         375  0.0108  0.7870  0.2022         375  0.0101  0.7878  0.2020
 400  0.0216  0.7741  0.2043         400  0.0202  0.7758  0.2040         400  0.0190  0.7772  0.2038
 425  0.0374  0.7552  0.2075         425  0.0349  0.7581  0.2070         425  0.0329  0.7605  0.2066
 450  0.0603  0.7276  0.2121         450  0.0565  0.7322  0.2113         450  0.0533  0.7360  0.2107
 475  0.0915  0.6902  0.2183         475  0.0860  0.6968  0.2172         475  0.0812  0.7025  0.2162
 500  0.1311  0.6427  0.2262         500  0.1236  0.6517  0.2247         500  0.1171  0.6594  0.2234
 525  0.1782  0.5861  0.2356         525  0.1687  0.5975  0.2337         525  0.1605  0.6074  0.2321
 550  0.2310  0.5228  0.2462         550  0.2197  0.5363  0.2439         550  0.2098  0.5482  0.2420
 575  0.2868  0.4558  0.2574         575  0.2741  0.4710  0.2548         575  0.2629  0.4845  0.2526
 600  0.3425  0.3890  0.2685         600  0.3291  0.4050  0.2658         600  0.3171  0.4194  0.2634
 625  0.3955  0.3254  0.2791         625  0.3820  0.3416  0.2764         625  0.3698  0.3562  0.2740
 650  0.4436  0.2677  0.2887         650  0.4306  0.2833  0.2861         650  0.4187  0.2975  0.2837
 675  0.4855  0.2174  0.2971         675  0.4735  0.2318  0.2947         675  0.4624  0.2451  0.2925
 700  0.5208  0.1750  0.3042         700  0.5101  0.1879  0.3020         700  0.5001  0.1999  0.3000
 725  0.5498  0.1402  0.3100         725  0.5405  0.1514  0.3081         725  0.5317  0.1620  0.3063
 750  0.5732  0.1121  0.3146         750  0.5652  0.1217  0.3130         750  0.5576  0.1308  0.3115
 775  0.5918  0.0898  0.3184         775  0.5851  0.0979  0.3170         775  0.5786  0.1057  0.3157
 800  0.6065  0.0722  0.3213         800  0.6009  0.0790  0.3202         800  0.5954  0.0855  0.3191
 825  0.6180  0.0583  0.3236         825  0.6133  0.0640  0.3227         825  0.6087  0.0695  0.3217
 850  0.6271  0.0474  0.3254         850  0.6232  0.0522  0.3246         850  0.6193  0.0568  0.3239
 875  0.6343  0.0388  0.3269         875  0.6310  0.0428  0.3262         875  0.6278  0.0467  0.3255
 900  0.6400  0.0320  0.3280         900  0.6372  0.0353  0.3274         900  0.6345  0.0386  0.3269
 925  0.6445  0.0266  0.3289         925  0.6421  0.0294  0.3284         925  0.6399  0.0322  0.3280
 950  0.6481  0.0223  0.3296         950  0.6461  0.0246  0.3292         950  0.6442  0.0270  0.3288
 975  0.6510  0.0188  0.3302         975  0.6493  0.0208  0.3299         975  0.6477  0.0228  0.3295
1000  0.6534  0.0160  0.3307        1000  0.6519  0.0177  0.3304        1000  0.6505  0.0194  0.3301
```

PRESSURE = 120.0 ATM.

TEMP	H2	NH3	N2
300	0.0008	0.7990	0.2002
325	0.0021	0.7975	0.2004
350	0.0047	0.7944	0.2009
375	0.0096	0.7885	0.2019
400	0.0179	0.7785	0.2036
425	0.0311	0.7627	0.2062
450	0.0505	0.7394	0.2101
475	0.0771	0.7075	0.2154
500	0.1115	0.6662	0.2223
525	0.1532	0.6161	0.2306
550	0.2010	0.5588	0.2402
575	0.2529	0.4965	0.2506
600	0.3063	0.4325	0.2612
625	0.3586	0.3696	0.2717
650	0.4077	0.3107	0.2815
675	0.4520	0.2576	0.2904
700	0.4906	0.2113	0.2981
725	0.5233	0.1721	0.3046
750	0.5503	0.1396	0.3101
775	0.5723	0.1132	0.3145
800	0.5901	0.0919	0.3180
825	0.6043	0.0749	0.3208
850	0.6156	0.0613	0.3231
875	0.6246	0.0505	0.3249
900	0.6318	0.0418	0.3264
925	0.6376	0.0349	0.3275
950	0.6423	0.0293	0.3284
975	0.6460	0.0247	0.3292
1000	0.6491	0.0211	0.3298

PRESSURE = 130.0 ATM.

TEMP	H2	NH3	N2
300	0.0008	0.7991	0.2001
325	0.0019	0.7977	0.2004
350	0.0044	0.7947	0.2009
375	0.0091	0.7891	0.2018
400	0.0170	0.7796	0.2034
425	0.0296	0.7645	0.2059
450	0.0480	0.7424	0.2096
475	0.0735	0.7118	0.2147
500	0.1065	0.6722	0.2213
525	0.1467	0.6239	0.2293
550	0.1931	0.5682	0.2386
575	0.2438	0.5074	0.2488
600	0.2964	0.4443	0.2593
625	0.3484	0.3820	0.2697
650	0.3976	0.3229	0.2795
675	0.4423	0.2692	0.2885
700	0.4817	0.2220	0.2963
725	0.5153	0.1817	0.3030
750	0.5433	0.1480	0.3087
775	0.5663	0.1205	0.3133
800	0.5849	0.0981	0.3170
825	0.5999	0.0801	0.3200
850	0.6119	0.0657	0.3224
875	0.6215	0.0542	0.3243
900	0.6292	0.0450	0.3258
925	0.6354	0.0376	0.3271
950	0.6404	0.0316	0.3281
975	0.6444	0.0267	0.3289
1000	0.6477	0.0227	0.3295

PRESSURE = 140.0 ATM.

TEMP	H2	NH3	N2
300	0.0007	0.7991	0.2001
325	0.0019	0.7978	0.2004
350	0.0042	0.7949	0.2008
375	0.0086	0.7896	0.2017
400	0.0162	0.7805	0.2032
425	0.0282	0.7662	0.2056
450	0.0458	0.7450	0.2092
475	0.0703	0.7157	0.2140
500	0.1020	0.6776	0.2204
525	0.1409	0.6309	0.2282
550	0.1860	0.5768	0.2372
575	0.2356	0.5173	0.2471
600	0.2873	0.4552	0.2575
625	0.3389	0.3933	0.2678
650	0.3881	0.3343	0.2776
675	0.4332	0.2801	0.2866
700	0.4732	0.2321	0.2946
725	0.5076	0.1908	0.3015
750	0.5366	0.1561	0.3073
775	0.5604	0.1275	0.3121
800	0.5799	0.1041	0.3160
825	0.5956	0.0853	0.3191
850	0.6083	0.0701	0.3216
875	0.6184	0.0579	0.3237
900	0.6266	0.0481	0.3253
925	0.6332	0.0402	0.3266
950	0.6385	0.0338	0.3277
975	0.6428	0.0286	0.3286
1000	0.6463	0.0244	0.3293

PRESSURE = 150.0 ATM.

TEMP	H2	NH3	N2
300	0.0007	0.7992	0.2001
325	0.0018	0.7979	0.2004
350	0.0040	0.7952	0.2008
375	0.0083	0.7901	0.2016
400	0.0155	0.7814	0.2031
425	0.0270	0.7676	0.2054
450	0.0439	0.7473	0.2088
475	0.0674	0.7191	0.2135
500	0.0980	0.6824	0.2196
525	0.1357	0.6372	0.2271
550	0.1796	0.5845	0.2359
575	0.2281	0.5263	0.2456
600	0.2790	0.4652	0.2558
625	0.3301	0.4038	0.2660
650	0.3793	0.3449	0.2758
675	0.4247	0.2904	0.2849
700	0.4652	0.2417	0.2930
725	0.5003	0.1996	0.3001
750	0.5301	0.1639	0.3060
775	0.5548	0.1343	0.3109
800	0.5750	0.1100	0.3150
825	0.5914	0.0903	0.3183
850	0.6047	0.0744	0.3209
875	0.6154	0.0615	0.3231
900	0.6240	0.0512	0.3248
925	0.6310	0.0428	0.3262
950	0.6366	0.0361	0.3273
975	0.6412	0.0305	0.3282
1000	0.6450	0.0260	0.3290

PRESSURE = 160.0 ATM.

TEMP	H2	NH3	N2
300	0.0007	0.7992	0.2001
325	0.0017	0.7980	0.2003
350	0.0039	0.7954	0.2008
375	0.0079	0.7905	0.2016
400	0.0149	0.7822	0.2030
425	0.0259	0.7690	0.2052
450	0.0422	0.7494	0.2084
475	0.0648	0.7222	0.2130
500	0.0944	0.6867	0.2189
525	0.1309	0.6429	0.2262
550	0.1737	0.5916	0.2347
575	0.2212	0.5346	0.2442
600	0.2713	0.4744	0.2543
625	0.3220	0.4136	0.2644
650	0.3710	0.3548	0.2742
675	0.4166	0.3001	0.2833
700	0.4576	0.2509	0.2915
725	0.4934	0.2080	0.2987
750	0.5238	0.1714	0.3048
775	0.5493	0.1409	0.3099
800	0.5702	0.1157	0.3140
825	0.5873	0.0952	0.3175
850	0.6012	0.0785	0.3202
875	0.6124	0.0651	0.3225
900	0.6215	0.0542	0.3243
925	0.6288	0.0454	0.3258
950	0.6348	0.0383	0.3269
975	0.6396	0.0324	0.3279
1000	0.6436	0.0277	0.3287

PRESSURE = 170.0 ATM.

TEMP	H2	NH3	N2
300	0.0006	0.7992	0.2001
325	0.0016	0.7980	0.2003
350	0.0037	0.7955	0.2007
375	0.0076	0.7909	0.2015
400	0.0143	0.7829	0.2029
425	0.0249	0.7701	0.2050
450	0.0406	0.7513	0.2081
475	0.0624	0.7251	0.2125
500	0.0911	0.6907	0.2182
525	0.1266	0.6481	0.2253
550	0.1683	0.5980	0.2337
575	0.2148	0.5422	0.2430
600	0.2642	0.4830	0.2528
625	0.3144	0.4227	0.2629
650	0.3632	0.3641	0.2726
675	0.4089	0.3093	0.2818
700	0.4503	0.2596	0.2901
725	0.4867	0.2160	0.2973
750	0.5178	0.1786	0.3036
775	0.5440	0.1472	0.3088
800	0.5656	0.1213	0.3131
825	0.5834	0.1000	0.3167
850	0.5978	0.0826	0.3196
875	0.6095	0.0686	0.3219
900	0.6190	0.0572	0.3238
925	0.6267	0.0480	0.3253
950	0.6329	0.0405	0.3266
975	0.6381	0.0343	0.3276
1000	0.6422	0.0293	0.3284

PRESSURE = 180.0 ATM.

TEMP	H2	NH3	N2
300	0.0006	0.7993	0.2001
325	0.0016	0.7981	0.2003
350	0.0036	0.7957	0.2007
375	0.0073	0.7912	0.2015
400	0.0138	0.7835	0.2027
425	0.0240	0.7712	0.2048
450	0.0391	0.7530	0.2078
475	0.0603	0.7277	0.2121
500	0.0881	0.6943	0.2176
525	0.1226	0.6529	0.2245
550	0.1633	0.6040	0.2327
575	0.2089	0.5493	0.2418
600	0.2576	0.4909	0.2515
625	0.3072	0.4313	0.2614
650	0.3559	0.3729	0.2712
675	0.4017	0.3180	0.2803
700	0.4434	0.2679	0.2887
725	0.4802	0.2237	0.2960
750	0.5120	0.1856	0.3024
775	0.5388	0.1534	0.3078
800	0.5611	0.1267	0.3122
825	0.5794	0.1047	0.3159
850	0.5944	0.0867	0.3189
875	0.6066	0.0721	0.3213
900	0.6165	0.0602	0.3233
925	0.6246	0.0505	0.3249
950	0.6311	0.0426	0.3262
975	0.6365	0.0362	0.3273
1000	0.6409	0.0309	0.3282

PRESSURE = 190.0 ATM.

TEMP	H2	NH3	N2
300	0.0006	0.7993	0.2001
325	0.0015	0.7982	0.2003
350	0.0034	0.7959	0.2007
375	0.0071	0.7915	0.2014
400	0.0133	0.7841	0.2027
425	0.0231	0.7722	0.2046
450	0.0378	0.7546	0.2076
475	0.0583	0.7300	0.2117
500	0.0853	0.6976	0.2171
525	0.1189	0.6573	0.2238
550	0.1587	0.6096	0.2317
575	0.2034	0.5559	0.2407
600	0.2514	0.4984	0.2503
625	0.3005	0.4393	0.2601
650	0.3489	0.3813	0.2698
675	0.3948	0.3262	0.2790
700	0.4368	0.2759	0.2874
725	0.4741	0.2311	0.2948
750	0.5064	0.1923	0.3013
775	0.5338	0.1594	0.3068
800	0.5567	0.1319	0.3113
825	0.5756	0.1092	0.3151
850	0.5911	0.0906	0.3182
875	0.6038	0.0755	0.3208
900	0.6141	0.0631	0.3228
925	0.6225	0.0530	0.3245
950	0.6293	0.0448	0.3259
975	0.6350	0.0380	0.3270
1000	0.6396	0.0325	0.3279

PRESSURE = 200.0 ATM.

TEMP	H2	NH3	N2
300	0.0006	0.7993	0.2001
325	0.0015	0.7982	0.2003
350	0.0033	0.7960	0.2007
375	0.0068	0.7918	0.2014
400	0.0128	0.7846	0.2026
425	0.0224	0.7731	0.2045
450	0.0366	0.7561	0.2073
475	0.0565	0.7322	0.2113
500	0.0827	0.7007	0.2165
525	0.1155	0.6614	0.2231
550	0.1544	0.6147	0.2309
575	0.1983	0.5620	0.2397
600	0.2455	0.5053	0.2491
625	0.2942	0.4469	0.2588
650	0.3424	0.3891	0.2685
675	0.3882	0.3341	0.2776
700	0.4304	0.2835	0.2861
725	0.4681	0.2382	0.2936
750	0.5009	0.1989	0.3002
775	0.5289	0.1653	0.3058
800	0.5524	0.1371	0.3105
825	0.5719	0.1137	0.3144
850	0.5879	0.0945	0.3176
875	0.6010	0.0788	0.3202
900	0.6117	0.0660	0.3223
925	0.6204	0.0555	0.3241
950	0.6276	0.0469	0.3255
975	0.6334	0.0399	0.3267
1000	0.6382	0.0341	0.3276

```
PRESSURE =  210.0 ATM.                  PRESSURE =  220.0 ATM.                  PRESSURE =  230.0 ATM.

TEMP    H2       NH3      N2            TEMP    H2       NH3      N2            TEMP    H2       NH3      N2
 300  0.0005   0.7993   0.2001           300  0.0005   0.7994   0.2001           300  0.0005   0.7994   0.2001
 325  0.0014   0.7983   0.2003           325  0.0014   0.7983   0.2003           325  0.0013   0.7984   0.2003
 350  0.0032   0.7961   0.2006           350  0.0031   0.7962   0.2006           350  0.0030   0.7963   0.2006
 375  0.0066   0.7921   0.2013           375  0.0064   0.7923   0.2013           375  0.0062   0.7925   0.2012
 400  0.0124   0.7851   0.2025           400  0.0121   0.7855   0.2024           400  0.0117   0.7859   0.2023
 425  0.0217   0.7740   0.2043           425  0.0211   0.7747   0.2042           425  0.0205   0.7754   0.2041
 450  0.0355   0.7574   0.2071           450  0.0345   0.7586   0.2069           450  0.0335   0.7598   0.2067
 475  0.0548   0.7342   0.2110           475  0.0533   0.7361   0.2106           475  0.0518   0.7378   0.2104
 500  0.0804   0.7036   0.2161           500  0.0782   0.7062   0.2156           500  0.0761   0.7087   0.2152
 525  0.1124   0.6652   0.2225           525  0.1094   0.6687   0.2219           525  0.1067   0.6720   0.2213
 550  0.1504   0.6195   0.2301           550  0.1467   0.6240   0.2293           550  0.1432   0.6282   0.2286
 575  0.1935   0.5678   0.2387           575  0.1890   0.5732   0.2378           575  0.1848   0.5782   0.2370
 600  0.2401   0.5119   0.2480           600  0.2350   0.5180   0.2470           600  0.2301   0.5239   0.2460
 625  0.2883   0.4540   0.2577           625  0.2827   0.4608   0.2565           625  0.2773   0.4672   0.2555
 650  0.3362   0.3966   0.2672           650  0.3303   0.4037   0.2661           650  0.3246   0.4104   0.2649
 675  0.3820   0.3416   0.2764           675  0.3760   0.3488   0.2752           675  0.3703   0.3556   0.2741
 700  0.4244   0.2907   0.2849           700  0.4185   0.2977   0.2837           700  0.4130   0.3044   0.2826
 725  0.4624   0.2451   0.2925           725  0.4569   0.2517   0.2914           725  0.4516   0.2581   0.2903
 750  0.4957   0.2052   0.2991           750  0.4906   0.2113   0.2981           750  0.4857   0.2172   0.2971
 775  0.5242   0.1710   0.3048           775  0.5196   0.1765   0.3039           775  0.5151   0.1818   0.3030
 800  0.5482   0.1421   0.3096           800  0.5441   0.1470   0.3088           800  0.5401   0.1518   0.3080
 825  0.5682   0.1181   0.3136           825  0.5646   0.1225   0.3129           825  0.5611   0.1267   0.3122
 850  0.5847   0.0984   0.3169           850  0.5816   0.1021   0.3163           850  0.5785   0.1058   0.3157
 875  0.5982   0.0821   0.3196           875  0.5955   0.0854   0.3191           875  0.5928   0.0886   0.3186
 900  0.6093   0.0688   0.3219           900  0.6070   0.0716   0.3214           900  0.6046   0.0744   0.3209
 925  0.6184   0.0579   0.3237           925  0.6163   0.0604   0.3233           925  0.6143   0.0628   0.3229
 950  0.6258   0.0490   0.3252           950  0.6241   0.0511   0.3248           950  0.6223   0.0532   0.3245
 975  0.6319   0.0417   0.3264           975  0.6304   0.0435   0.3261           975  0.6289   0.0453   0.3258
1000  0.6369   0.0357   0.3274          1000  0.6356   0.0372   0.3271          1000  0.6343   0.0388   0.3269
```

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PRESSURE =  240.0 ATM.               PRESSURE =  250.0 ATM.               PRESSURE =  260.0 ATM.

TEMP    H2      NH3      N2          TEMP    H2      NH3      N2          TEMP    H2      NH3      N2
 300  0.0005  0.7994  0.2001          300  0.0005  0.7994  0.2001          300  0.0005  0.7994  0.2001
 325  0.0013  0.7984  0.2003          325  0.0013  0.7985  0.2002          325  0.0012  0.7985  0.2002
 350  0.0030  0.7964  0.2006          350  0.0029  0.7965  0.2006          350  0.0028  0.7966  0.2006
 375  0.0061  0.7927  0.2012          375  0.0059  0.7929  0.2012          375  0.0057  0.7931  0.2011
 400  0.0114  0.7863  0.2023          400  0.0111  0.7867  0.2022          400  0.0108  0.7870  0.2022
 425  0.0199  0.7761  0.2040          425  0.0194  0.7767  0.2039          425  0.0189  0.7773  0.2038
 450  0.0326  0.7609  0.2065          450  0.0318  0.7619  0.2063          450  0.0310  0.7628  0.2062
 475  0.0505  0.7394  0.2101          475  0.0492  0.7410  0.2098          475  0.0480  0.7424  0.2096
 500  0.0742  0.7110  0.2148          500  0.0724  0.7131  0.2145          500  0.0707  0.7152  0.2141
 525  0.1041  0.6751  0.2208          525  0.1016  0.6780  0.2203          525  0.0994  0.6808  0.2199
 550  0.1399  0.6321  0.2280          550  0.1368  0.6358  0.2274          550  0.1339  0.6393  0.2268
 575  0.1808  0.5830  0.2362          575  0.1771  0.5875  0.2354          575  0.1735  0.5918  0.2347
 600  0.2255  0.5294  0.2451          600  0.2212  0.5346  0.2442          600  0.2170  0.5396  0.2434
 625  0.2723  0.4733  0.2544          625  0.2674  0.4790  0.2535          625  0.2629  0.4846  0.2526
 650  0.3193  0.4168  0.2639          650  0.3142  0.4230  0.2628          650  0.3093  0.4289  0.2618
 675  0.3649  0.3622  0.2730          675  0.3596  0.3684  0.2719          675  0.3546  0.3745  0.2709
 700  0.4076  0.3109  0.2815          700  0.4024  0.3171  0.2805          700  0.3974  0.3231  0.2795
 725  0.4464  0.2643  0.2893          725  0.4415  0.2702  0.2883          725  0.4367  0.2760  0.2873
 750  0.4809  0.2229  0.2962          750  0.4762  0.2285  0.2952          750  0.4717  0.2339  0.2943
 775  0.5108  0.1871  0.3021          775  0.5065  0.1922  0.3013          775  0.5024  0.1971  0.3005
 800  0.5362  0.1565  0.3072          800  0.5324  0.1611  0.3065          800  0.5287  0.1656  0.3057
 825  0.5576  0.1308  0.3115          825  0.5542  0.1349  0.3108          825  0.5509  0.1389  0.3102
 850  0.5755  0.1094  0.3151          850  0.5725  0.1130  0.3145          850  0.5696  0.1165  0.3139
 875  0.5902  0.0917  0.3180          875  0.5876  0.0949  0.3175          875  0.5851  0.0979  0.3170
 900  0.6024  0.0771  0.3205          900  0.6001  0.0799  0.3200          900  0.5979  0.0825  0.3196
 925  0.6124  0.0651  0.3225          925  0.6104  0.0675  0.3221          925  0.6085  0.0698  0.3217
 950  0.6206  0.0553  0.3241          950  0.6189  0.0573  0.3238          950  0.6172  0.0593  0.3234
 975  0.6274  0.0471  0.3255          975  0.6259  0.0489  0.3252          975  0.6245  0.0506  0.3249
1000  0.6330  0.0404  0.3266         1000  0.6317  0.0419  0.3263         1000  0.6305  0.0434  0.3261
```

PRESSURE = 270.0 ATM.

TEMP	H2	NH3	N2
300	0.0005	0.7994	0.2001
325	0.0012	0.7986	0.2002
350	0.0027	0.7967	0.2005
375	0.0056	0.7933	0.2011
400	0.0105	0.7873	0.2021
425	0.0184	0.7779	0.2037
450	0.0302	0.7637	0.2060
475	0.0469	0.7437	0.2094
500	0.0691	0.7171	0.2138
525	0.0972	0.6834	0.2194
550	0.1311	0.6427	0.2262
575	0.1701	0.5958	0.2340
600	0.2131	0.5443	0.2426
625	0.2585	0.4898	0.2517
650	0.3046	0.4345	0.2609
675	0.3498	0.3803	0.2699
700	0.3926	0.3289	0.2785
725	0.4320	0.2816	0.2864
750	0.4673	0.2392	0.2935
775	0.4983	0.2020	0.2997
800	0.5250	0.1700	0.3050
825	0.5477	0.1428	0.3095
850	0.5667	0.1200	0.3133
875	0.5825	0.1010	0.3165
900	0.5957	0.0852	0.3191
925	0.6066	0.0721	0.3213
950	0.6156	0.0613	0.3231
975	0.6230	0.0524	0.3246
1000	0.6292	0.0449	0.3258

PRESSURE = 280.0 ATM.

TEMP	H2	NH3	N2
300	0.0004	0.7994	0.2001
325	0.0012	0.7986	0.2002
350	0.0027	0.7968	0.2005
375	0.0055	0.7934	0.2011
400	0.0103	0.7876	0.2021
425	0.0180	0.7784	0.2036
450	0.0295	0.7645	0.2059
475	0.0458	0.7450	0.2092
500	0.0676	0.7189	0.2135
525	0.0952	0.6858	0.2190
550	0.1285	0.6458	0.2257
575	0.1669	0.5997	0.2334
600	0.2093	0.5488	0.2419
625	0.2543	0.4948	0.2509
650	0.3001	0.4399	0.2600
675	0.3451	0.3859	0.2690
700	0.3879	0.3345	0.2776
725	0.4275	0.2870	0.2855
750	0.4631	0.2443	0.2926
775	0.4944	0.2067	0.2989
800	0.5214	0.1743	0.3043
825	0.5445	0.1466	0.3089
850	0.5638	0.1234	0.3128
875	0.5800	0.1039	0.3160
900	0.5935	0.0878	0.3187
925	0.6047	0.0744	0.3209
950	0.6139	0.0633	0.3228
975	0.6216	0.0541	0.3243
1000	0.6280	0.0464	0.3256

PRESSURE = 290.0 ATM.

TEMP	H2	NH3	N2
300	0.0004	0.7995	0.2001
325	0.0011	0.7986	0.2002
350	0.0026	0.7969	0.2005
375	0.0053	0.7936	0.2011
400	0.0101	0.7879	0.2020
425	0.0176	0.7789	0.2035
450	0.0289	0.7653	0.2058
475	0.0448	0.7462	0.2090
500	0.0661	0.7206	0.2132
525	0.0932	0.6881	0.2186
550	0.1260	0.6488	0.2252
575	0.1639	0.6034	0.2328
600	0.2058	0.5531	0.2412
625	0.2503	0.4996	0.2501
650	0.2958	0.4451	0.2591
675	0.3406	0.3912	0.2681
700	0.3834	0.3399	0.2767
725	0.4231	0.2922	0.2846
750	0.4589	0.2493	0.2918
775	0.4905	0.2113	0.2981
800	0.5179	0.1785	0.3036
825	0.5413	0.1504	0.3083
850	0.5611	0.1267	0.3122
875	0.5776	0.1069	0.3155
900	0.5914	0.0904	0.3183
925	0.6028	0.0766	0.3206
950	0.6123	0.0653	0.3225
975	0.6202	0.0558	0.3240
1000	0.6267	0.0479	0.3253

PRESSURE = 300.0 ATM.

TEMP	H2	NH3	N2
300	0.0004	0.7995	0.2001
325	0.0011	0.7987	0.2002
350	0.0025	0.7969	0.2005
375	0.0052	0.7937	0.2010
400	0.0098	0.7882	0.2020
425	0.0172	0.7793	0.2034
450	0.0283	0.7661	0.2056
475	0.0439	0.7473	0.2088
500	0.0648	0.7222	0.2130
525	0.0914	0.6903	0.2183
550	0.1236	0.6516	0.2247
575	0.1610	0.6068	0.2322
600	0.2024	0.5572	0.2405
625	0.2464	0.5043	0.2493
650	0.2916	0.4500	0.2583
675	0.3363	0.3964	0.2673
700	0.3791	0.3451	0.2758
725	0.4189	0.2973	0.2838
750	0.4549	0.2541	0.2910
775	0.4868	0.2158	0.2974
800	0.5145	0.1826	0.3029
825	0.5382	0.1541	0.3076
850	0.5583	0.1300	0.3117
875	0.5752	0.1098	0.3150
900	0.5892	0.0929	0.3178
925	0.6009	0.0789	0.3202
950	0.6107	0.0672	0.3221
975	0.6187	0.0575	0.3237
1000	0.6255	0.0494	0.3251

PRESSURE = 310.0 ATM.

TEMP	H2	NH3	N2
300	0.0004	0.7995	0.2001
325	0.0011	0.7987	0.2002
350	0.0025	0.7970	0.2005
375	0.0051	0.7939	0.2010
400	0.0096	0.7884	0.2019
425	0.0168	0.7798	0.2034
450	0.0277	0.7668	0.2055
475	0.0430	0.7484	0.2086
500	0.0635	0.7238	0.2127
525	0.0896	0.6924	0.2179
550	0.1214	0.6544	0.2243
575	0.1582	0.6102	0.2316
600	0.1991	0.5611	0.2398
625	0.2428	0.5087	0.2485
650	0.2876	0.4548	0.2575
675	0.3321	0.4014	0.2664
700	0.3749	0.3501	0.2750
725	0.4147	0.3023	0.2829
750	0.4510	0.2588	0.2902
775	0.4831	0.2203	0.2966
800	0.5111	0.1866	0.3022
825	0.5352	0.1577	0.3070
850	0.5556	0.1333	0.3111
875	0.5728	0.1127	0.3146
900	0.5871	0.0954	0.3174
925	0.5991	0.0811	0.3198
950	0.6090	0.0691	0.3218
975	0.6173	0.0592	0.3235
1000	0.6242	0.0509	0.3248

PRESSURE = 320.0 ATM.

TEMP	H2	NH3	N2
300	0.0004	0.7995	0.2001
325	0.0011	0.7987	0.2002
350	0.0024	0.7971	0.2005
375	0.0050	0.7940	0.2010
400	0.0094	0.7887	0.2019
425	0.0165	0.7802	0.2033
450	0.0271	0.7675	0.2054
475	0.0421	0.7494	0.2084
500	0.0623	0.7253	0.2125
525	0.0880	0.6944	0.2176
550	0.1192	0.6569	0.2238
575	0.1555	0.6134	0.2311
600	0.1960	0.5648	0.2392
625	0.2392	0.5129	0.2478
650	0.2838	0.4594	0.2568
675	0.3281	0.4062	0.2656
700	0.3708	0.3550	0.2742
725	0.4107	0.3071	0.2821
750	0.4471	0.2634	0.2894
775	0.4795	0.2246	0.2959
800	0.5078	0.1906	0.3016
825	0.5322	0.1613	0.3064
850	0.5529	0.1365	0.3106
875	0.5704	0.1155	0.3141
900	0.5850	0.0979	0.3170
925	0.5973	0.0833	0.3194
950	0.6074	0.0710	0.3215
975	0.6159	0.0609	0.3232
1000	0.6230	0.0524	0.3246

PRESSURE = 330.0 ATM.

TEMP	H2	NH3	N2
300	0.0004	0.7995	0.2001
325	0.0010	0.7987	0.2002
350	0.0024	0.7971	0.2005
375	0.0049	0.7941	0.2010
400	0.0092	0.7889	0.2018
425	0.0162	0.7806	0.2032
450	0.0266	0.7681	0.2053
475	0.0413	0.7504	0.2083
500	0.0611	0.7267	0.2122
525	0.0864	0.6963	0.2173
550	0.1172	0.6594	0.2234
575	0.1530	0.6164	0.2306
600	0.1930	0.5684	0.2386
625	0.2358	0.5170	0.2472
650	0.2801	0.4639	0.2560
675	0.3242	0.4109	0.2648
700	0.3669	0.3597	0.2734
725	0.4068	0.3118	0.2814
750	0.4434	0.2679	0.2887
775	0.4760	0.2288	0.2952
800	0.5046	0.1944	0.3009
825	0.5293	0.1648	0.3059
850	0.5503	0.1396	0.3101
875	0.5681	0.1183	0.3136
900	0.5830	0.1004	0.3166
925	0.5955	0.0854	0.3191
950	0.6059	0.0729	0.3212
975	0.6145	0.0625	0.3229
1000	0.6218	0.0538	0.3244

PRESSURE = 340.0 ATM.

TEMP	H2	NH3	N2
300	0.0004	0.7995	0.2001
325	0.0010	0.7988	0.2002
350	0.0023	0.7972	0.2005
375	0.0048	0.7942	0.2010
400	0.0091	0.7891	0.2018
425	0.0159	0.7810	0.2032
450	0.0261	0.7687	0.2052
475	0.0406	0.7513	0.2081
500	0.0600	0.7280	0.2120
525	0.0849	0.6981	0.2170
550	0.1152	0.6618	0.2230
575	0.1505	0.6193	0.2301
600	0.1901	0.5719	0.2380
625	0.2326	0.5209	0.2465
650	0.2765	0.4682	0.2553
675	0.3205	0.4154	0.2641
700	0.3630	0.3643	0.2726
725	0.4031	0.3163	0.2806
750	0.4397	0.2723	0.2879
775	0.4726	0.2329	0.2945
800	0.5015	0.1982	0.3003
825	0.5264	0.1683	0.3053
850	0.5477	0.1427	0.3095
875	0.5658	0.1210	0.3132
900	0.5810	0.1028	0.3162
925	0.5937	0.0876	0.3187
950	0.6043	0.0748	0.3209
975	0.6132	0.0642	0.3226
1000	0.6206	0.0553	0.3241

PRESSURE = 350.0 ATM.

TEMP	H2	NH3	N2
300	0.0004	0.7995	0.2001
325	0.0010	0.7988	0.2002
350	0.0023	0.7972	0.2005
375	0.0047	0.7943	0.2009
400	0.0089	0.7893	0.2018
425	0.0156	0.7813	0.2031
450	0.0256	0.7693	0.2051
475	0.0398	0.7522	0.2080
500	0.0589	0.7293	0.2118
525	0.0834	0.6999	0.2167
550	0.1133	0.6640	0.2227
575	0.1482	0.6221	0.2296
600	0.1873	0.5752	0.2375
625	0.2294	0.5247	0.2459
650	0.2731	0.4723	0.2546
675	0.3168	0.4198	0.2634
700	0.3593	0.3688	0.2719
725	0.3994	0.3207	0.2799
750	0.4362	0.2766	0.2872
775	0.4692	0.2369	0.2938
800	0.4983	0.2020	0.2997
825	0.5236	0.1717	0.3047
850	0.5452	0.1458	0.3090
875	0.5635	0.1238	0.3127
900	0.5790	0.1052	0.3158
925	0.5919	0.0897	0.3184
950	0.6027	0.0767	0.3205
975	0.6118	0.0658	0.3224
1000	0.6194	0.0567	0.3239

PRESSURE = 360.0 ATM.

TEMP	H2	NH3	N2
300	0.0004	0.7995	0.2001
325	0.0010	0.7988	0.2002
350	0.0023	0.7973	0.2004
375	0.0046	0.7944	0.2009
400	0.0087	0.7895	0.2017
425	0.0153	0.7817	0.2031
450	0.0251	0.7698	0.2050
475	0.0391	0.7531	0.2078
500	0.0579	0.7305	0.2116
525	0.0820	0.7016	0.2164
550	0.1115	0.6662	0.2223
575	0.1460	0.6248	0.2292
600	0.1846	0.5784	0.2369
625	0.2264	0.5284	0.2453
650	0.2697	0.4763	0.2539
675	0.3133	0.4240	0.2627
700	0.3557	0.3731	0.2711
725	0.3958	0.3250	0.2792
750	0.4327	0.2807	0.2865
775	0.4659	0.2409	0.2932
800	0.4953	0.2056	0.2991
825	0.5208	0.1750	0.3042
850	0.5427	0.1488	0.3085
875	0.5613	0.1264	0.3123
900	0.5770	0.1076	0.3154
925	0.5902	0.0918	0.3180
950	0.6012	0.0785	0.3202
975	0.6105	0.0674	0.3221
1000	0.6182	0.0582	0.3236

PRESSURE = 370.0 ATM.

TEMP	H2	NH3	N2
300	0.0004	0.7995	0.2001
325	0.0010	0.7988	0.2002
350	0.0022	0.7973	0.2004
375	0.0045	0.7945	0.2009
400	0.0086	0.7897	0.2017
425	0.0150	0.7820	0.2030
450	0.0247	0.7704	0.2049
475	0.0384	0.7539	0.2077
500	0.0570	0.7316	0.2114
525	0.0807	0.7031	0.2161
550	0.1098	0.6683	0.2219
575	0.1438	0.6274	0.2288
600	0.1821	0.5815	0.2364
625	0.2234	0.5319	0.2447
650	0.2665	0.4802	0.2533
675	0.3099	0.4281	0.2620
700	0.3522	0.3774	0.2704
725	0.3923	0.3292	0.2785
750	0.4293	0.2848	0.2859
775	0.4627	0.2447	0.2925
800	0.4923	0.2092	0.2985
825	0.5181	0.1783	0.3036
850	0.5402	0.1517	0.3080
875	0.5591	0.1291	0.3118
900	0.5750	0.1100	0.3150
925	0.5884	0.0939	0.3177
950	0.5997	0.0804	0.3199
975	0.6091	0.0691	0.3218
1000	0.6170	0.0596	0.3234

PRESSURE = 380.0 ATM.

TEMP	H2	NH3	N2
300	0.0004	0.7995	0.2001
325	0.0010	0.7988	0.2002
350	0.0022	0.7974	0.2004
375	0.0045	0.7946	0.2009
400	0.0084	0.7899	0.2017
425	0.0147	0.7823	0.2029
450	0.0243	0.7709	0.2048
475	0.0378	0.7546	0.2076
500	0.0560	0.7328	0.2112
525	0.0794	0.7047	0.2159
550	0.1081	0.6703	0.2216
575	0.1417	0.6299	0.2283
600	0.1796	0.5845	0.2359
625	0.2206	0.5353	0.2441
650	0.2634	0.4839	0.2527
675	0.3066	0.4321	0.2613
700	0.3488	0.3815	0.2698
725	0.3889	0.3333	0.2778
750	0.4260	0.2888	0.2852
775	0.4596	0.2485	0.2919
800	0.4894	0.2127	0.2979
825	0.5154	0.1815	0.3031
850	0.5378	0.1547	0.3076
875	0.5569	0.1317	0.3114
900	0.5731	0.1123	0.3146
925	0.5867	0.0959	0.3173
950	0.5982	0.0822	0.3196
975	0.6078	0.0707	0.3215
1000	0.6158	0.0610	0.3232

PRESSURE = 390.0 ATM.

TEMP	H2	NH3	N2
300	0.0004	0.7996	0.2001
325	0.0009	0.7989	0.2002
350	0.0021	0.7974	0.2004
375	0.0044	0.7947	0.2009
400	0.0083	0.7901	0.2017
425	0.0145	0.7826	0.2029
450	0.0239	0.7713	0.2048
475	0.0372	0.7554	0.2074
500	0.0551	0.7338	0.2110
525	0.0782	0.7061	0.2156
550	0.1065	0.6722	0.2213
575	0.1397	0.6323	0.2279
600	0.1772	0.5873	0.2354
625	0.2179	0.5386	0.2436
650	0.2604	0.4875	0.2521
675	0.3033	0.4360	0.2607
700	0.3455	0.3854	0.2691
725	0.3856	0.3373	0.2771
750	0.4228	0.2927	0.2845
775	0.4565	0.2522	0.2913
800	0.4865	0.2162	0.2973
825	0.5127	0.1847	0.3025
850	0.5354	0.1575	0.3071
875	0.5547	0.1343	0.3109
900	0.5711	0.1146	0.3142
925	0.5850	0.0980	0.3170
950	0.5966	0.0840	0.3193
975	0.6064	0.0723	0.3213
1000	0.6147	0.0624	0.3229

PRESSURE = 400.0 ATM.

TEMP	H2	NH3	N2
300	0.0004	0.7996	0.2001
325	0.0009	0.7989	0.2002
350	0.0021	0.7975	0.2004
375	0.0043	0.7948	0.2009
400	0.0081	0.7902	0.2016
425	0.0143	0.7829	0.2028
450	0.0235	0.7718	0.2047
475	0.0366	0.7561	0.2073
500	0.0543	0.7349	0.2109
525	0.0770	0.7076	0.2154
550	0.1050	0.6740	0.2210
575	0.1378	0.6346	0.2276
600	0.1749	0.5901	0.2350
625	0.2152	0.5417	0.2430
650	0.2574	0.4911	0.2515
675	0.3002	0.4397	0.2600
700	0.3422	0.3893	0.2684
725	0.3823	0.3412	0.2765
750	0.4196	0.2965	0.2839
775	0.4535	0.2558	0.2907
800	0.4837	0.2196	0.2967
825	0.5101	0.1879	0.3020
850	0.5330	0.1604	0.3066
875	0.5526	0.1369	0.3105
900	0.5692	0.1169	0.3138
925	0.5833	0.1000	0.3167
950	0.5952	0.0858	0.3190
975	0.6051	0.0738	0.3210
1000	0.6135	0.0638	0.3227

PRESSURE = 410.0 ATM.

TEMP	H2	NH3	N2
300	0.0003	0.7996	0.2001
325	0.0009	0.7989	0.2002
350	0.0021	0.7975	0.2004
375	0.0042	0.7949	0.2008
400	0.0080	0.7904	0.2016
425	0.0140	0.7832	0.2028
450	0.0231	0.7723	0.2046
475	0.0360	0.7568	0.2072
500	0.0535	0.7358	0.2107
525	0.0759	0.7089	0.2152
550	0.1035	0.6758	0.2207
575	0.1360	0.6368	0.2272
600	0.1727	0.5928	0.2345
625	0.2126	0.5448	0.2425
650	0.2546	0.4945	0.2509
675	0.2972	0.4434	0.2594
700	0.3391	0.3931	0.2678
725	0.3791	0.3450	0.2758
750	0.4165	0.3002	0.2833
775	0.4505	0.2594	0.2901
800	0.4809	0.2229	0.2962
825	0.5075	0.1909	0.3015
850	0.5307	0.1632	0.3061
875	0.5505	0.1394	0.3101
900	0.5674	0.1192	0.3135
925	0.5816	0.1020	0.3163
950	0.5937	0.0876	0.3187
975	0.6038	0.0754	0.3208
1000	0.6123	0.0652	0.3225

```
PRESSURE =  420.0 ATM.            PRESSURE =  430.0 ATM.            PRESSURE =  440.0 ATM.

TEMP    H2      NH3     N2        TEMP    H2      NH3     N2        TEMP    H2      NH3     N2
 300  0.0003  0.7996  0.2001       300  0.0003  0.7996  0.2001       300  0.0003  0.7996  0.2001
 325  0.0009  0.7989  0.2002       325  0.0009  0.7989  0.2002       325  0.0009  0.7990  0.2002
 350  0.0020  0.7976  0.2004       350  0.0020  0.7976  0.2004       350  0.0020  0.7976  0.2004
 375  0.0042  0.7950  0.2008       375  0.0041  0.7951  0.2008       375  0.0041  0.7951  0.2008
 400  0.0079  0.7905  0.2016       400  0.0078  0.7907  0.2015       400  0.0076  0.7908  0.2015
 425  0.0138  0.7834  0.2028       425  0.0136  0.7837  0.2027       425  0.0134  0.7839  0.2027
 450  0.0227  0.7727  0.2045       450  0.0224  0.7731  0.2045       450  0.0221  0.7735  0.2044
 475  0.0355  0.7574  0.2071       475  0.0349  0.7581  0.2070       475  0.0344  0.7587  0.2069
 500  0.0527  0.7368  0.2105       500  0.0519  0.7377  0.2104       500  0.0512  0.7386  0.2102
 525  0.0748  0.7102  0.2150       525  0.0737  0.7115  0.2147       525  0.0727  0.7127  0.2145
 550  0.1020  0.6775  0.2204       550  0.1007  0.6792  0.2201       550  0.0993  0.6808  0.2199
 575  0.1342  0.6390  0.2268       575  0.1324  0.6411  0.2265       575  0.1307  0.6431  0.2261
 600  0.1705  0.5954  0.2341       600  0.1684  0.5979  0.2337       600  0.1664  0.6003  0.2333
 625  0.2102  0.5478  0.2420       625  0.2078  0.5507  0.2415       625  0.2054  0.5535  0.2411
 650  0.2518  0.4978  0.2504       650  0.2492  0.5010  0.2498       650  0.2466  0.5041  0.2493
 675  0.2942  0.4469  0.2588       675  0.2913  0.4504  0.2583       675  0.2886  0.4537  0.2577
 700  0.3360  0.3968  0.2672       700  0.3330  0.4004  0.2666       700  0.3301  0.4039  0.2660
 725  0.3761  0.3487  0.2752       725  0.3730  0.3524  0.2746       725  0.3701  0.3559  0.2740
 750  0.4134  0.3039  0.2827       750  0.4105  0.3074  0.2821       750  0.4076  0.3109  0.2815
 775  0.4476  0.2629  0.2895       775  0.4447  0.2663  0.2889       775  0.4419  0.2697  0.2884
 800  0.4781  0.2262  0.2956       800  0.4754  0.2295  0.2951       800  0.4728  0.2326  0.2946
 825  0.5050  0.1940  0.3010       825  0.5025  0.1970  0.3005       825  0.5001  0.1999  0.3000
 850  0.5284  0.1660  0.3057       850  0.5261  0.1687  0.3052       850  0.5238  0.1714  0.3048
 875  0.5484  0.1419  0.3097       875  0.5464  0.1444  0.3093       875  0.5443  0.1468  0.3089
 900  0.5655  0.1214  0.3131       900  0.5637  0.1236  0.3127       900  0.5618  0.1258  0.3124
 925  0.5800  0.1040  0.3160       925  0.5783  0.1060  0.3157       925  0.5767  0.1079  0.3153
 950  0.5922  0.0893  0.3184       950  0.5908  0.0911  0.3181       950  0.5893  0.0928  0.3179
 975  0.6025  0.0770  0.3205       975  0.6012  0.0785  0.3202       975  0.5999  0.0801  0.3200
1000  0.6112  0.0666  0.3222      1000  0.6101  0.0679  0.3220      1000  0.6089  0.0693  0.3218
```

PRESSURE = 450.0 ATM.

TEMP	H2	NH3	N2
300	0.0003	0.7996	0.2001
325	0.0009	0.7990	0.2002
350	0.0019	0.7977	0.2004
375	0.0040	0.7952	0.2008
400	0.0075	0.7910	0.2015
425	0.0132	0.7841	0.2026
450	0.0218	0.7739	0.2043
475	0.0339	0.7593	0.2068
500	0.0504	0.7395	0.2101
525	0.0717	0.7139	0.2143
550	0.0980	0.6824	0.2196
575	0.1291	0.6450	0.2258
600	0.1645	0.6026	0.2329
625	0.2032	0.5562	0.2406
650	0.2440	0.5071	0.2488
675	0.2858	0.4570	0.2572
700	0.3273	0.4073	0.2654
725	0.3672	0.3594	0.2734
750	0.4047	0.3143	0.2809
775	0.4392	0.2730	0.2878
800	0.4702	0.2357	0.2940
825	0.4977	0.2028	0.2995
850	0.5216	0.1740	0.3043
875	0.5423	0.1492	0.3085
900	0.5600	0.1280	0.3120
925	0.5751	0.1099	0.3150
950	0.5879	0.0945	0.3176
975	0.5987	0.0816	0.3197
1000	0.6078	0.0706	0.3216

PRESSURE = 460.0 ATM.

TEMP	H2	NH3	N2
300	0.0003	0.7996	0.2001
325	0.0008	0.7990	0.2002
350	0.0019	0.7977	0.2004
375	0.0039	0.7953	0.2008
400	0.0074	0.7911	0.2015
425	0.0130	0.7844	0.2026
450	0.0214	0.7742	0.2043
475	0.0335	0.7598	0.2067
500	0.0498	0.7403	0.2099
525	0.0708	0.7150	0.2142
550	0.0968	0.6839	0.2194
575	0.1276	0.6469	0.2255
600	0.1626	0.6049	0.2325
625	0.2010	0.5588	0.2402
650	0.2416	0.5101	0.2483
675	0.2832	0.4602	0.2566
700	0.3245	0.4106	0.2649
725	0.3644	0.3627	0.2729
750	0.4019	0.3177	0.2804
775	0.4365	0.2762	0.2873
800	0.4676	0.2388	0.2935
825	0.4953	0.2057	0.2991
850	0.5194	0.1767	0.3039
875	0.5403	0.1516	0.3081
900	0.5582	0.1301	0.3116
925	0.5735	0.1118	0.3147
950	0.5864	0.0962	0.3173
975	0.5974	0.0831	0.3195
1000	0.6067	0.0720	0.3213

PRESSURE = 470.0 ATM.

TEMP	H2	NH3	N2
300	0.0003	0.7996	0.2001
325	0.0008	0.7990	0.2002
350	0.0019	0.7977	0.2004
375	0.0039	0.7953	0.2008
400	0.0073	0.7912	0.2015
425	0.0128	0.7846	0.2026
450	0.0212	0.7746	0.2042
475	0.0330	0.7604	0.2066
500	0.0491	0.7411	0.2098
525	0.0699	0.7161	0.2140
550	0.0956	0.6853	0.2191
575	0.1260	0.6488	0.2252
600	0.1607	0.6071	0.2321
625	0.1988	0.5614	0.2398
650	0.2392	0.5130	0.2478
675	0.2806	0.4633	0.2561
700	0.3218	0.4139	0.2644
725	0.3616	0.3661	0.2723
750	0.3992	0.3210	0.2798
775	0.4338	0.2794	0.2868
800	0.4651	0.2418	0.2930
825	0.4929	0.2085	0.2986
850	0.5173	0.1792	0.3035
875	0.5384	0.1539	0.3077
900	0.5565	0.1322	0.3113
925	0.5719	0.1137	0.3144
950	0.5850	0.0979	0.3170
975	0.5962	0.0846	0.3192
1000	0.6056	0.0733	0.3211

```
PRESSURE =  480.0 ATM.            PRESSURE =  490.0 ATM.            PRESSURE =  500.0 ATM.

TEMP    H2      NH3     N2        TEMP    H2      NH3     N2        TEMP    H2      NH3     N2
 300  0.0003  0.7996  0.2001       300  0.0003  0.7996  0.2001       300  0.0003  0.7996  0.2001
 325  0.0008  0.7990  0.2002       325  0.0008  0.7990  0.2002       325  0.0008  0.7990  0.2002
 350  0.0019  0.7978  0.2004       350  0.0018  0.7978  0.2004       350  0.0018  0.7978  0.2004
 375  0.0038  0.7954  0.2008       375  0.0038  0.7955  0.2007       375  0.0037  0.7955  0.2007
 400  0.0072  0.7913  0.2014       400  0.0071  0.7915  0.2014       400  0.0070  0.7916  0.2014
 425  0.0127  0.7848  0.2025       425  0.0125  0.7850  0.2025       425  0.0123  0.7852  0.2025
 450  0.0209  0.7749  0.2042       450  0.0206  0.7753  0.2041       450  0.0203  0.7756  0.2041
 475  0.0326  0.7609  0.2065       475  0.0322  0.7614  0.2064       475  0.0317  0.7619  0.2063
 500  0.0485  0.7418  0.2097       500  0.0478  0.7426  0.2096       500  0.0472  0.7433  0.2094
 525  0.0690  0.7172  0.2138       525  0.0681  0.7182  0.2136       525  0.0673  0.7192  0.2135
 550  0.0944  0.6867  0.2189       550  0.0933  0.6881  0.2186       550  0.0922  0.6894  0.2184
 575  0.1246  0.6505  0.2249       575  0.1231  0.6522  0.2246       575  0.1217  0.6539  0.2243
 600  0.1589  0.6093  0.2318       600  0.1572  0.6113  0.2314       600  0.1555  0.6134  0.2311
 625  0.1967  0.5639  0.2393       625  0.1947  0.5663  0.2389       625  0.1928  0.5687  0.2385
 650  0.2369  0.5158  0.2474       650  0.2346  0.5185  0.2469       650  0.2324  0.5211  0.2465
 675  0.2781  0.4663  0.2556       675  0.2756  0.4693  0.2551       675  0.2732  0.4722  0.2546
 700  0.3191  0.4170  0.2638       700  0.3165  0.4201  0.2633       700  0.3140  0.4232  0.2628
 725  0.3589  0.3693  0.2718       725  0.3563  0.3725  0.2712       725  0.3537  0.3756  0.2707
 750  0.3965  0.3242  0.2793       750  0.3939  0.3273  0.2788       750  0.3913  0.3304  0.2783
 775  0.4312  0.2825  0.2862       775  0.4287  0.2856  0.2857       775  0.4262  0.2886  0.2852
 800  0.4627  0.2448  0.2925       800  0.4602  0.2477  0.2920       800  0.4578  0.2506  0.2916
 825  0.4906  0.2112  0.2981       825  0.4883  0.2140  0.2977       825  0.4861  0.2167  0.2972
 850  0.5152  0.1818  0.3030       850  0.5131  0.1843  0.3026       850  0.5110  0.1868  0.3022
 875  0.5364  0.1563  0.3073       875  0.5345  0.1586  0.3069       875  0.5326  0.1608  0.3065
 900  0.5547  0.1343  0.3109       900  0.5530  0.1364  0.3106       900  0.5513  0.1385  0.3103
 925  0.5704  0.1156  0.3141       925  0.5688  0.1174  0.3138       925  0.5673  0.1193  0.3134
 950  0.5836  0.0996  0.3167       950  0.5822  0.1013  0.3164       950  0.5809  0.1029  0.3162
 975  0.5949  0.0861  0.3190       975  0.5937  0.0876  0.3187       975  0.5924  0.0891  0.3185
1000  0.6045  0.0746  0.3209      1000  0.6034  0.0760  0.3207      1000  0.6023  0.0773  0.3204
```

```
PRESSURE =  510.0 ATM.

TEMP     H2      NH3      N2
 300   0.0003  0.7996  0.2001
 325   0.0008  0.7991  0.2002
 350   0.0018  0.7978  0.2004
 375   0.0037  0.7956  0.2007
 400   0.0069  0.7917  0.2014
 425   0.0122  0.7854  0.2024
 450   0.0201  0.7759  0.2040
 475   0.0313  0.7624  0.2063
 500   0.0467  0.7440  0.2093
 525   0.0665  0.7202  0.2133
 550   0.0911  0.6907  0.2182
 575   0.1204  0.6555  0.2241
 600   0.1539  0.6153  0.2308
 625   0.1908  0.5710  0.2382
 650   0.2302  0.5237  0.2460
 675   0.2708  0.4750  0.2542
 700   0.3115  0.4262  0.2623
 725   0.3511  0.3786  0.2702
 750   0.3888  0.3335  0.2777
 775   0.4237  0.2916  0.2847
 800   0.4555  0.2534  0.2911
 825   0.4839  0.2193  0.2968
 850   0.5089  0.1893  0.3018
 875   0.5307  0.1631  0.3061
 900   0.5496  0.1405  0.3099
 925   0.5657  0.1211  0.3131
 950   0.5795  0.1046  0.3159
 975   0.5912  0.0905  0.3182
1000   0.6012  0.0786  0.3202
```

```
PRESSURE =  520.0 ATM.

TEMP     H2      NH3      N2
 300   0.0003  0.7996  0.2001
 325   0.0008  0.7991  0.2002
 350   0.0018  0.7979  0.2003
 375   0.0036  0.7956  0.2007
 400   0.0068  0.7918  0.2014
 425   0.0120  0.7856  0.2024
 450   0.0198  0.7762  0.2040
 475   0.0310  0.7628  0.2062
 500   0.0461  0.7447  0.2092
 525   0.0657  0.7211  0.2131
 550   0.0901  0.6919  0.2180
 575   0.1191  0.6571  0.2238
 600   0.1523  0.6172  0.2305
 625   0.1890  0.5732  0.2378
 650   0.2281  0.5262  0.2456
 675   0.2686  0.4777  0.2537
 700   0.3091  0.4291  0.2618
 725   0.3487  0.3816  0.2697
 750   0.3863  0.3365  0.2773
 775   0.4213  0.2945  0.2842
 800   0.4531  0.2562  0.2906
 825   0.4817  0.2220  0.2963
 850   0.5069  0.1917  0.3014
 875   0.5289  0.1653  0.3058
 900   0.5479  0.1425  0.3096
 925   0.5642  0.1229  0.3128
 950   0.5781  0.1062  0.3156
 975   0.5900  0.0920  0.3180
1000   0.6001  0.0799  0.3200
```

```
PRESSURE =  530.0 ATM.

TEMP     H2      NH3      N2
 300   0.0003  0.7996  0.2001
 325   0.0008  0.7991  0.2001
 350   0.0017  0.7979  0.2003
 375   0.0036  0.7957  0.2007
 400   0.0068  0.7919  0.2013
 425   0.0119  0.7858  0.2024
 450   0.0196  0.7765  0.2039
 475   0.0306  0.7633  0.2061
 500   0.0455  0.7453  0.2091
 525   0.0650  0.7220  0.2130
 550   0.0891  0.6931  0.2178
 575   0.1178  0.6586  0.2236
 600   0.1507  0.6191  0.2301
 625   0.1872  0.5754  0.2374
 650   0.2261  0.5287  0.2452
 675   0.2663  0.4804  0.2533
 700   0.3067  0.4319  0.2613
 725   0.3462  0.3845  0.2692
 750   0.3838  0.3394  0.2768
 775   0.4189  0.2973  0.2838
 800   0.4508  0.2590  0.2902
 825   0.4795  0.2245  0.2959
 850   0.5049  0.1941  0.3010
 875   0.5271  0.1675  0.3054
 900   0.5462  0.1445  0.3092
 925   0.5627  0.1247  0.3125
 950   0.5768  0.1078  0.3154
 975   0.5888  0.0934  0.3178
1000   0.5990  0.0812  0.3198
```

PRESSURE = 540.0 ATM.

TEMP	H2	NH3	N2
300	0.0003	0.7996	0.2001
325	0.0008	0.7991	0.2001
350	0.0017	0.7979	0.2003
375	0.0035	0.7957	0.2007
400	0.0067	0.7920	0.2013
425	0.0117	0.7859	0.2023
450	0.0193	0.7768	0.2039
475	0.0302	0.7637	0.2060
500	0.0450	0.7460	0.2090
525	0.0642	0.7229	0.2128
550	0.0881	0.6943	0.2176
575	0.1166	0.6601	0.2233
600	0.1492	0.6209	0.2298
625	0.1854	0.5775	0.2371
650	0.2241	0.5311	0.2448
675	0.2641	0.4830	0.2528
700	0.3044	0.4347	0.2609
725	0.3438	0.3874	0.2688
750	0.3814	0.3423	0.2763
775	0.4165	0.3002	0.2833
800	0.4486	0.2617	0.2897
825	0.4774	0.2271	0.2955
850	0.5029	0.1965	0.3006
875	0.5252	0.1697	0.3050
900	0.5446	0.1465	0.3089
925	0.5612	0.1265	0.3122
950	0.5755	0.1094	0.3151
975	0.5876	0.0949	0.3175
1000	0.5979	0.0825	0.3196

PRESSURE = 550.0 ATM.

TEMP	H2	NH3	N2
300	0.0003	0.7996	0.2001
325	0.0007	0.7991	0.2001
350	0.0017	0.7980	0.2003
375	0.0035	0.7958	0.2007
400	0.0066	0.7921	0.2013
425	0.0116	0.7861	0.2023
450	0.0191	0.7771	0.2038
475	0.0299	0.7642	0.2060
500	0.0445	0.7466	0.2089
525	0.0635	0.7238	0.2127
550	0.0871	0.6954	0.2174
575	0.1153	0.6616	0.2231
600	0.1478	0.6227	0.2295
625	0.1837	0.5796	0.2367
650	0.2221	0.5335	0.2444
675	0.2620	0.4856	0.2524
700	0.3021	0.4374	0.2604
725	0.3415	0.3902	0.2683
750	0.3791	0.3451	0.2758
775	0.4142	0.3029	0.2828
800	0.4464	0.2643	0.2893
825	0.4753	0.2296	0.2951
850	0.5010	0.1988	0.3002
875	0.5234	0.1719	0.3047
900	0.5429	0.1485	0.3086
925	0.5597	0.1283	0.3119
950	0.5741	0.1110	0.3148
975	0.5864	0.0963	0.3173
1000	0.5969	0.0837	0.3194

PRESSURE = 560.0 ATM.

TEMP	H2	NH3	N2
300	0.0003	0.7997	0.2001
325	0.0007	0.7991	0.2001
350	0.0017	0.7980	0.2003
375	0.0035	0.7958	0.2007
400	0.0065	0.7922	0.2013
425	0.0114	0.7863	0.2023
450	0.0189	0.7773	0.2038
475	0.0295	0.7646	0.2059
500	0.0440	0.7472	0.2088
525	0.0628	0.7246	0.2126
550	0.0862	0.6965	0.2172
575	0.1142	0.6630	0.2228
600	0.1463	0.6244	0.2293
625	0.1820	0.5816	0.2364
650	0.2202	0.5357	0.2440
675	0.2599	0.4881	0.2520
700	0.2999	0.4401	0.2600
725	0.3392	0.3930	0.2678
750	0.3768	0.3479	0.2754
775	0.4119	0.3057	0.2824
800	0.4442	0.2670	0.2888
825	0.4732	0.2321	0.2946
850	0.4990	0.2011	0.2998
875	0.5217	0.1740	0.3043
900	0.5413	0.1504	0.3083
925	0.5583	0.1301	0.3116
950	0.5728	0.1126	0.3146
975	0.5852	0.0977	0.3170
1000	0.5958	0.0850	0.3192

```
PRESSURE =  570.0 ATM.          PRESSURE =  580.0 ATM.          PRESSURE =  590.0 ATM.

TEMP    H2      NH3     N2      TEMP    H2      NH3     N2      TEMP    H2      NH3     N2
 300  0.0003  0.7997  0.2001     300  0.0003  0.7997  0.2001     300  0.0003  0.7997  0.2000
 325  0.0007  0.7991  0.2001     325  0.0007  0.7991  0.2001     325  0.0007  0.7991  0.2001
 350  0.0017  0.7980  0.2003     350  0.0016  0.7980  0.2003     350  0.0016  0.7980  0.2003
 375  0.0034  0.7959  0.2007     375  0.0034  0.7959  0.2007     375  0.0033  0.7960  0.2007
 400  0.0064  0.7923  0.2013     400  0.0064  0.7924  0.2013     400  0.0063  0.7924  0.2013
 425  0.0113  0.7864  0.2023     425  0.0112  0.7866  0.2022     425  0.0111  0.7867  0.2022
 450  0.0187  0.7776  0.2037     450  0.0185  0.7778  0.2037     450  0.0182  0.7781  0.2036
 475  0.0292  0.7650  0.2058     475  0.0289  0.7654  0.2058     475  0.0285  0.7657  0.2057
 500  0.0435  0.7478  0.2087     500  0.0430  0.7483  0.2086     500  0.0426  0.7489  0.2085
 525  0.0621  0.7254  0.2124     525  0.0615  0.7262  0.2123     525  0.0608  0.7270  0.2122
 550  0.0853  0.6976  0.2171     550  0.0844  0.6987  0.2169     550  0.0836  0.6997  0.2167
 575  0.1130  0.6644  0.2226     575  0.1119  0.6657  0.2224     575  0.1108  0.6670  0.2222
 600  0.1449  0.6261  0.2290     600  0.1436  0.6277  0.2287     600  0.1422  0.6293  0.2284
 625  0.1803  0.5836  0.2361     625  0.1787  0.5855  0.2357     625  0.1772  0.5874  0.2354
 650  0.2183  0.5380  0.2437     650  0.2165  0.5402  0.2433     650  0.2147  0.5423  0.2429
 675  0.2578  0.4906  0.2516     675  0.2558  0.4930  0.2512     675  0.2539  0.4953  0.2508
 700  0.2977  0.4427  0.2595     700  0.2956  0.4453  0.2591     700  0.2935  0.4478  0.2587
 725  0.3369  0.3957  0.2674     725  0.3347  0.3983  0.2669     725  0.3326  0.4009  0.2665
 750  0.3745  0.3506  0.2749     750  0.3723  0.3533  0.2745     750  0.3701  0.3559  0.2740
 775  0.4097  0.3083  0.2819     775  0.4075  0.3110  0.2815     775  0.4053  0.3136  0.2811
 800  0.4420  0.2696  0.2884     800  0.4399  0.2721  0.2880     800  0.4378  0.2746  0.2876
 825  0.4712  0.2346  0.2942     825  0.4692  0.2370  0.2938     825  0.4672  0.2394  0.2934
 850  0.4971  0.2034  0.2994     850  0.4952  0.2057  0.2990     850  0.4934  0.2079  0.2987
 875  0.5199  0.1761  0.3040     875  0.5182  0.1782  0.3036     875  0.5164  0.1803  0.3033
 900  0.5397  0.1523  0.3079     900  0.5381  0.1542  0.3076     900  0.5365  0.1561  0.3073
 925  0.5568  0.1318  0.3114     925  0.5554  0.1335  0.3111     925  0.0003  0.7997  0.2000
 950  0.5715  0.1142  0.3143     950  0.5702  0.1158  0.3140     950  0.5539  0.1353  0.3108
 975  0.5841  0.0991  0.3168     975  0.5829  0.1005  0.3166     975  0.5689  0.1173  0.3138
1000  0.5948  0.0863  0.3190    1000  0.5937  0.0875  0.3187    1000  0.5817  0.1019  0.3163
```

```
PRESSURE =  600.0 ATM.                PRESSURE =  610.0 ATM.

TEMP    H2       NH3      N2          TEMP    H2       NH3      N2
 300  0.5927   0.0888   0.3185         300  0.0003   0.7997   0.2000
 325  0.0007   0.7991   0.2001         325  0.0007   0.7992   0.2001
 350  0.0016   0.7981   0.2003         350  0.0016   0.7981   0.2003
 375  0.0033   0.7960   0.2007         375  0.0033   0.7961   0.2006
 400  0.0062   0.7925   0.2012         400  0.0062   0.7926   0.2012
 425  0.0109   0.7869   0.2022         425  0.0108   0.7870   0.2022
 450  0.0180   0.7783   0.2036         450  0.0179   0.7786   0.2036
 475  0.0282   0.7661   0.2056         475  0.0279   0.7665   0.2056
 500  0.0421   0.7494   0.2084         500  0.0417   0.7500   0.2083
 525  0.0602   0.7277   0.2120         525  0.0596   0.7285   0.2119
 550  0.0827   0.7007   0.2165         550  0.0819   0.7017   0.2164
 575  0.1098   0.6683   0.2219         575  0.1087   0.6695   0.2217
 600  0.1409   0.6309   0.2282         600  0.1397   0.6324   0.2279
 625  0.1756   0.5892   0.2351         625  0.1741   0.5910   0.2348
 650  0.2130   0.5444   0.2426         650  0.2113   0.5465   0.2423
 675  0.2520   0.4976   0.2504         675  0.2501   0.4999   0.2500
 700  0.2915   0.4502   0.2583         700  0.2895   0.4526   0.2579
 725  0.3304   0.4035   0.2661         725  0.3283   0.4060   0.2657
 750  0.3679   0.3585   0.2736         750  0.3658   0.3610   0.2732
 775  0.4032   0.3161   0.2806         775  0.4011   0.3187   0.2802
 800  0.4357   0.2771   0.2871         800  0.4337   0.2796   0.2867
 825  0.4652   0.2417   0.2930         825  0.4633   0.2441   0.2927
 850  0.4915   0.2101   0.2983         850  0.4897   0.2123   0.2979
 875  0.5147   0.1823   0.3029         875  0.5130   0.1843   0.3026
 900  0.5350   0.1580   0.3070         900  0.5334   0.1599   0.3067
 925  0.5525   0.1370   0.3105         925  0.5511   0.1386   0.3102
 950  0.5676   0.1188   0.3135         950  0.5664   0.1204   0.3133
 975  0.5806   0.1033   0.3161         975  0.5794   0.1047   0.3159
1000  0.5917   0.0900   0.3183        1000  0.5906   0.0912   0.3181
```