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Thermodynamic Properties of Ammonia as an Ideal Gas

Lester Haar

Institute for Basic Standards
National Bureau of Standards
Washington, D.C. 20234

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A. V. Astin, *Director.*

Contents

Thermodynamic Properties of Ammonia as an Ideal Gas*

Lester Haar

Institute for Basic Standards, National Bureau of Standards, Washington, D.C. 20234

(December 15, 1967)

Thermodynamic functions for ammonia as an ideal gas at one atmosphere pressure have been evaluated. The contribution of the highly anharmonic out-of-plane vibrational mode, including its large coupling with rotation and its coupling with the other vibrational modes, is considered in detail. Tables of C_p°/R, $(H^\circ - E_0^\circ)/RT$, $(E_0^\circ - G^\circ)/RT$, and S°/R have been calculated at closely spaced intervals from 50 to 5000 °K within an overall uncertainty of less than 0.1 percent at 1000 °K.

Key Words: Ammonia, ideal gas, thermodynamic functions.

1. Introduction

This paper is part of a program originating with the Office of Standard Reference Data of the National Bureau of Standards to obtain accurate thermodynamic properties for ammonia. Subsequent papers of this program will include real-gas corrections to the ideal-gas properties contained herein.

In this paper the ideal-gas thermodynamic properties of ammonia in the ground electronic state are calculated at closely spaced temperature intervals from 50 to 5000 °K. The calculations include the contributions of ordinary vibrational anharmonicity and vibrational-rotational coupling together with rotational stretching and rotational quantum effects. Particular attention is given to the treatment of the rotational and vibrational anharmonic effects due to the molecular inversion. To this end a method is developed for calculating this contribution such that an overall accuracy for the thermodynamic properties of ammonia approaching that of the simplest diatomic molecules is obtained.

In the vibrational ground state ammonia is a pyramidal molecule with the nitrogen atom approximately 0.38 Å above the plane of the three hydrogen atoms. The distance between the nitrogen atom and each of the hydrogen atoms is approximately 1.0 Å. Thus the pyramid is relatively flat and the potential barrier to vibration of the nitrogen atom through the plane of the hydrogen atoms so as to invert the pyramid is low (approximately 2000 cm^{-1} [1]).[1]

Ammonia has six vibrational degrees of freedom. However, owing to symmetry there are only four normal vibrational modes, two of which have double degeneracies. The vibrational structure may thus be characterized by the six quantum numbers $(v_1 v_2 v_3^{l_3} v_4^{l_4})$, where the v_i are the principal vibrational quantum numbers associated with the vibrational modes ν_i and the l characterize the small coupling of the degenerate ν_3 and ν_4 asymmetric vibrational modes with the angular momentum of the molecule. The ν_1 and ν_2 modes are symmetric, nondegenerate vibrations corresponding to stretching the N-H bond and spreading the pyramid, respectively. (The ν_2 mode is also referred to as the out-of-plane vibration.) The rotational structure for the ground state is that of a symmetric top, so that the rotational energy levels are characterized by the two quantum numbers J and K.

The ν_2 mode is the vibration associated with the inversion of the pyramid. Each vibrational state of this mode is split into two components, corresponding respectively to symmetric and antisymmetric eigenfunctions. (In the nomenclature these are identified by the superscript "s" or "a" to the quantum number v_2.) The spacing of these levels is highly anharmonic except for vibrational energies sufficiently higher or lower than the potential barrier to inversion. Thus the vibrational levels for the ground state of the ν_2 mode are only slightly split, of the order of a fraction of a wavenumber, but the splitting increases rapidly with increasing vibrational quantum number. At energy levels sufficiently elevated above the barrier (greater than about 3000 cm^{-1}) the levels become uniformly spaced with a spacing of approximately half that of the ν_2 fundamental. Similarly, due to inversion the rotational structure undergoes a transition from that of a pyramid for the low values of the v_2 quantum number to that of a planar molecule for the higher values, so that the rotational motion is also strongly coupled to the ν_2 mode. For a more detailed discussion of these effects, see the review by Herzberg [2] of the pyramidal XY_3 molecule and Nielsen [3]. The energy structure

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*This work was supported in part by the Office of Standard Reference Data, NBS.

[1] Figures in brackets indicate the literature references at the end of this paper.

of the other vibrational modes is similar to that of typical, slightly anharmonic rotating vibrators.

In section 2 the equations for the calculations are developed. This is followed in section 3 by a discussion of the molecular data, and in section 4 by a discussion of the calculated properties and an evaluation of their accuracy. Finally, a discussion is given in section 5 of some of the earlier work.

2. Partition Function

It is convenient to represent the rotational and vibrational structure by an expression for which the energy levels of the ν_2 mode and its coupling with the other degrees of freedom are written explicitly. Thus the energy levels in wavenumbers are written

$$T(v, J, K) = G'(v) + F'(v, J, K) + G_2(v, J, K), \tag{1}$$

where the primes denote that dependence on v_2 is omitted. The first term in eq (1) describes the vibrational energy characterized by $(v_1 0 v_3^{l_3} v_4^{l_4})$ and in notation similar to that in Herzberg [2] is approximated by

$$G'(v) = \sum_i{}' v_i \nu_i + \sum_{i>j} x_{ij} v_i v_j + \sum_i{}' x_{ii}(v_i - 1)v_i \ + \ldots$$

$$+ g_{34} l_3 l_4 + g_{33}(l_3^2 - v_3) + g_{44}(l_4^2 - v_4) + \ldots, \tag{2}$$

$$i, j \neq 2,$$

where the ν_i are fundamentals and the x and g are relatively small anharmonicities. The second term in eq (1) is approximated by

$$F'(v, J, K) = B'_v J(J+1) + (C'_v - B'_v)K^2 \tag{3}$$

$$- D_v^{J\prime} J^2 (J+1)^2 - D_v^{JK\prime} J(J+1)K^2 - D_v^{K\prime} K^4 + \ldots,$$

where C_v is the rotational constant corresponding to rotation about the symmetry axis and B_v is the constant for axes perpendicular to the symmetry axis. The quantities D_v^J, D_v^{JK}, and D_v^K are small coefficients associated with centrifugal distortion of the molecule. The subscript v to each of the coefficients of eq (3) indicate dependence or coupling with the vibrational motion. The primes indicate that dependence on v_2 is omitted; that is, the rotational constants of eq (3) are evaluated for v_2 equal to zero. The coupling of the rotational motion to vibrations other than the ν_2 mode is relatively small and is included here only to first order in the fundamentals.

$$B'_v = B_0 - \sum_i{}' \alpha_i^B v_i +$$

$$C'_v = C_0 - \sum_i{}' \alpha_i^C v_i +, \qquad i \neq 2$$

where B_0 and C_0 are rotational constants, and the α are small corrections. All coordinates involving the ν_2 mode, including its coupling with the other degrees of freedom are included in G_2. Thus G_2 includes those effects characterized by

$$(v_1 v_2 v_3^{l_3} v_4^{l_4} JK) - (v_1 0 v_3^{l_3} v_4^{l_4} JK).$$

The partition function for the rotational and vibrational structure may be written

$$Q = \sum_{v,J,K} \exp\{-T(v, J, K)c_2/T\}, \tag{4}$$

where $T(v, J, K)$ is discussed in eqs (1), (2), and (3). c_2 is the second radiation constant and T is the absolute temperature. The sum extends over all rotational and vibrational degrees of freedom including all values of the v, J, K quantum numbers. In the evaluation of eq (4) the contributions of the vibrational anharmonicity and vibration-rotation coupling effects contained in eqs (2) and (3) are all to be accounted for to first order; that is, only terms linear in x, g, and α are retained. Though G_2 is not conveniently described by the usual power series in the vibrational quantum numbers, its contribution, including coupling effects with the other degrees of freedom, is also to be included to this order.

The contribution of the G_2 term is obtained by expanding the partition function about the term-by-term sum of the observed $(0v_2 00)$ energy levels. This summation incorporates the major effect of the highly anharmonic ν_2 mode, which is the coupling between the symmetric and antisymmetric states, but it does not include the contribution of the ν_2 coupling with the other vibrational modes. From an examination of the spectroscopic vibrational data (see Benedict et al. [4]), it can be seen that this cross coupling produces a shifting of energy levels of about the same magnitude as that of the other vibrational couplings (those represented by the x and g terms in eq (2)). Thus the contribution to the partition function of this cross coupling should be of the same order as that from the other anharmonicities, and a first order approximation for this contribution should be adequate.

In the expansion that follows expressions for the cross coupling are developed and their contribution for each individual $(0v_2 00)$ state obtained explicitly. The cross coupling between a pair of vibrational states, e.g., states corresponding to the particular quantum numbers v_1 and v_2, is defined as

$$G_{v_1 v_2} \equiv G(v_1 v_2 00) - G(v_1 000) - G(0 v_2 00), \tag{5}$$

where $G(v_1 v_2 v_3^{l_3} v_4^{l_4})$ is the vibrational energy. A useful representation for the coupling involving the highly anharmonic ν_2 mode is the development of $G_{v_1 v_2}$ as a power series of products of the observed energies, that is

$$G_{v_1 v_2} = k_{12} G(v_1 000) \cdot G(0 v_2 00) + \ldots \tag{6}$$

The constant k_{12} is readily determined in terms of the observed coupling. Thus for coupling between the fundamentals the observed coupling x_{12} is given by

$$
\begin{aligned}
x_{12} &= k_{12}G(1000)\cdot G(0100) \qquad + \ldots \\
&= k_{12}\nu_1\nu_2 + \ldots .
\end{aligned}
$$

Note that eq (6) reduces identically to the power series of eq (2) when the cross coupling is between nearly harmonic modes.

Consider the energy of the nearly harmonic oscillator ν_m, neglecting all anharmonicities but the cross coupling with ν_2. The energy levels for such an oscillator are given by

$$G_m = \nu_m v_m + G_{v_m v_2}.$$

Substituting from eq (6) and defining $E_2 \equiv G(0v_200)$, this becomes

$$G_m \cong \nu_m v_m + k_{2m}\nu_m v_m \cdot E_2. \tag{7}$$

The contribution of G_m to the partition function is the factor

$$Q_m = \left\{\sum_{v_m} \exp - \left[(c_2/T)\,(\nu_m v_m + k_{2m}E_2\nu_m v_m) \right]\right\}^{d_m}, \tag{8}$$

where d_m is the degeneracy of the mth mode. The anharmonicity term in the exponential of eq (8) is now expanded and only the linear term retained to yield

$$Q_m = \left\{\sum_{v_m} \left\{\exp\left[-\frac{c_2}{T}\,\nu_m v_m\right]\right\}\left\{1-\frac{c_2}{T}\,k_{2m}\nu_m v_m E_2\right\}\right\}^{d_m}. \tag{9}$$

Using the identity

$$-\frac{d}{d\alpha}\sum_v e^{-\alpha v} = \sum_v v e^{-\alpha v},$$

the contribution of Q_m becomes

$$Q_m = \left(1-e^{-\frac{c_2}{T}\nu_m}\right)^{-d_m}\left(1-f_{2m}\right), \tag{10}$$

where

$$f_{2m} = d_m \frac{c_2}{T}\,k_{2m}E_2\nu_m/\left(e^{c_2\nu_m/T}-1\right). \tag{11}$$

The factor $(1-f_{2m})$ is the contribution of the interaction of a particular $(0v_200)$ energy state with the mth vibrational mode, and it depends explicitly on E_2. It is clear then that the effect of this coupling is to modify each of the terms in the term-by-term sum over the $(0v_200)$ energy levels by the factor $(1-f_{2m})$. The term-by-term sum including cross coupling with the other vibrational modes is thus given by

$$Q_{v_2}\,(\text{vib}) = \sum_{E_2}\prod_m{}' \,(1-f_{2m})\,\exp\,(-c_2E_2/T). \tag{12}$$

The prime indicates that the $m=2$ factor in the product corresponding to self coupling of the ν_2 mode is omitted.

The coupling of rotation with the ν_2 mode is included by evaluating the classical rotational partition function for each of the $(0v_200)$ energy levels and employing these as separate weighting factors to each of the terms in eq (12). These factors are the usual expression for a classical nonrigid rotator,

$$Q_R(v_2) = \pi^{1/2}(\sigma_B^2\sigma_C)^{-1/2}(1+\rho^{(1)}T+\rho^{(2)}T^2). \tag{13}$$

The quantities σ_B and σ_C are given by,

$$\sigma_B = \frac{c_2}{T}\,B_{v_2},$$

$$\sigma_C = \frac{c_2}{T}\,C_{v_2},$$

where B_{v_2} and C_{v_2} are the observed rotational constants for the particular $(0v_200)$ energy level. The factor $1+\rho^{(1)}T+\rho^{(2)}T^2$ is the contribution of rotational stretching (see, for example (5 and 14)), where the ρ are calculated from the rotational stretching coefficients that apply to the particular $(0v_200)$ level.

One further simplification is required in order to evaluate the out-of-plane contribution. This is to obtain an approximation for the contribution of the energy levels corresponding to high values of the v_2 quantum number. Note that the ν_2 mode is nearly harmonic for energies corresponding to the fourth quantum number and higher, so that the contribution of these levels may be replaced by the well-known expression for a slightly anharmonic rotating vibrator. Combining eqs (12) and (13) and including the closed form approximation for the contribution of the states corresponding to quantum numbers given by $v_2 > 3$ yields the expression for $G_2\ (v,\ J,\ K)$ used in this calculation.

$$
\begin{aligned}
Q_{v_2} = \Bigg\{ &\sum_{v_2<4} \frac{B_0}{B_E}\left(\frac{C_0}{C_E}\right)^{1/2}(1+\rho^{(1)}T+\rho^{(2)}T^2)\,\cdot \\
&\qquad \prod_j{}' \,(1-f_{2j})\,e^{-\frac{c_2}{T}E}\Bigg\} \\
&+\frac{\exp\,(-c_2E_{4s}/T)}{1-\exp\,(-c_2\nu_2'/T)}\cdot\frac{B_0}{B_4}\left(\frac{C_0}{C_4}\right)^{1/2}\cdot \\
&\qquad \prod_j\,(1-\theta_{2j})\,(1+\phi_2)\,(1+\rho^{(1)}T),
\end{aligned}
\tag{14}
$$

where $E \equiv E_2$ and the subscript to E now refers to the particular v_2 quantum number. The quantity in the braces in eq (14) includes levels only up to $v_2 = 3^a$. Note that the rigid rotational contribution for the ground state has been factored from eq (14). In the second term the factor $\dfrac{\exp\,(-c_2E_{4s}/T)}{1-\exp\,(-c_2\nu_2'/T)}$ is the harmonic oscillator contribution with E_{4s} as the first level and ν_2' the fundamental. The factor $1-\theta_{2j}$ is the ordinary anharmonicity coupling with the jth vibrational mode, where

$$\theta_{ij}=\frac{\frac{c_2}{T}x_{ij}d_id_j}{(\exp(c_2\nu_i/T)-1)(\exp(c_2\nu_j/T)-1)},$$

$$\theta_{ii}=\frac{\frac{c_2}{T}(x_{ii}-g_{ii}/3)d_i(d_i+1)}{(\exp(c_2\nu_i/T)-1)^2}. \tag{15a}$$

The factor $1+\phi_2$ is the well-known contribution of rotation-vibration coupling, where

$$\phi_i=d_i\left(\frac{\alpha_i^B}{B}+\frac{1}{2}\frac{\alpha_i^C}{C}\right). \tag{15b}$$

Details concerning the derivation of quantities in eqs (15) may be found in Friedman and Haar [6], Woolley [7], and Pennington and Kobe [8], for example.

The contributions to the partition function of the two remaining terms $G'(v, J, K)$ and $F'(v, J, K)$ are quite straightforward (see [6, 7, 8]). With these the complete partition function is finally obtained.

$$Q=\frac{1}{S}\prod_{m=1}^{4}{}'\,(1-e^{-\frac{c_2}{T}\nu_m})^{-d_m}\prod_{i\leq j}^{4}{}'\,(1-\theta_{ij})\prod_{k=1}^{4}{}'\,(1+\phi_k)$$

$$\left(\frac{\Pi}{\sigma_{B_0}^2\sigma_{C_0}}\right)^{1/2}\cdot Q_{v_2}\cdot Q_{\mathrm{tr}}\cdot Q_{qr}. \tag{16}$$

As noted earlier the primes on the product summations indicate that factors containing the vibrational coordinate v_2 are omitted. The quantity S is the symmetry number. For the usual symmetric top molecule this has the value three. However, each of the components of the nondegenerate but split $(0v_200)$ levels have been counted with a statistical weight of unity, so that the factor Q_{v_2} is larger by a factor of two. This error is corrected by setting $S=6$. (Incidentally $S=6$ corresponds to the symmetry for a planar configuration for NH_3, and eq (16) might be thought of as an expansion about this planar configuration.) The product over m is the harmonic oscillator contribution for the modes other than ν_2; the products over ij and over k are the corresponding anharmonicity and rotation-vibration coupling contributions, respectively. The degeneracy coefficients d are unity for $m=1, 2$, and two for $m=3, 4$. The θ_{ij} and ϕ_k are given by eq (15). Q_{tr} is the usual contribution of translation. Lastly, the factor Q_{qr} is a correction for rotational quantum effects. It is very small at temperatures for which the vibrations are appreciably excited, so that it is not coupled to the ν_2 mode. The contribution Q_{qr} is given by Stripp and Kirkwood [9] for an asymmetric rotator, which for a symmetric top rotator reduces to

$$Q_{qr}=1+\frac{\sigma_B}{3}\left(1-\frac{1}{4}\frac{\sigma_B}{\sigma_C}\right)+\frac{\sigma_B^2}{15}\left(1-\frac{3}{4}\frac{\sigma_B}{\sigma_C}+\frac{7}{32}\frac{\sigma_B^2}{\sigma_C^2}\right).$$

3. Molecular Data

The molecular data upon which the calculations are based are listed in tables 1 and 2. Table 1 lists the data sensitive to the inversion coordinates and utilized in the term-by-term sum (the quantity in braces in eq (14)). The vibrational energies corresponding to $v_2=0, 3$ are from [4]. The energies corresponding to $v_2=1, 2$ are from Garing et al. [10]. The values listed for the rotational constants B_v and C_v corresponding to the $v_2=0$ states are from [4]; those corresponding to the $v_2=1, 2$ states from [10]; and to the $v_2=3$ states from Benedict et al. [11]. The rotational stretching constants D_v^J, D_v^{JK}, D_v^K are the average of the symmetric and antisymmetric values. The values for $v_2=0$ are from [4]; for $v_2=1$, from [10]; for $v_2=3$, from [11]; finally, data for $v_2=2$ were taken equal to the $v_2=1$ values.

TABLE 1. *The out-of-plane molecular constants in cm^{-1},* $v_2\leqslant 3$, $(0v_200)$

State	0^s	0^a	1^s	1^a	2^s	2^a	3^s	3^a
ν_2	0.0	0.793	932.41	968.04	1597.42	1882.16	2383.46	2895.48
B_{v_2}	9.9443	9.939	10.07	9.89	10.26	9.73	9.50	9.20
C_{v_2}	6.196	6.198	6.05	6.13	5.90	6.13	6.16	6.26
$D_{v_2}^J$	8.1×10^{-4}		8.9×10^{-4}		8.9×10^{-4}		-3.3×10^{-4}	
$D_{v_2}^{JK}$	-14.5×10^{-4}		-17.5×10^{-4}		-17.5×10^{-4}		15.0×10^{-4}	
$D_{v_2}^K$	7.5×10^{-4}		10.5×10^{-4}		10.5×10^{-4}		-11.3×10^{-4}	

TABLE 2. *Vibrational, rotational and coupling constants in cm^{-1}; see eqs (2), (3)*

$\nu_1(1\ 0\ 0\ 0)$	$\nu_2'=E_{4a}-E_{4s}$	$\nu_3(0\ 0\ 1\ 0)$	$\nu_4(0\ 0\ 0\ 1)$
3323.06	475	3443.381	1627.77
$x_{11}=-30$	$x_{22}=+9$	$x_{33}=-18.5$	$x_{44}=-8.8$
$x_{12}=+20.6$	$x_{23}=+32.36$	$x_{34}=-17.3$	$g_{44}=+2.65$
$x_{13}=-92$	$x_{24}=-10.7$		
$x_{14}=-6.7$	$B_4=9.35$, $C_4=6.21$		
$\alpha_1^B=0.135$	$\alpha_2^B=+0.015$	$\alpha_3^B=+0.176$	$\alpha_4^B=-0.230$
$\alpha_1^C=$ .078	$\alpha_2^C=+0.098$	$\alpha_3^C=-0.009$	$\alpha_4^C=+0.066$

The remaining molecular data are given in table 2. The vibrational fundamental ν_1 is from Benedict et al. [12]; ν_3 is from [11]; ν_4 is from [10]. The constants $\nu_2'$and x_{22} which correspond to the high energy, nearly-harmonic region of the ν_2 mode are derived from the reported values for the (04^s00) and (05^s00) levels at 3330 cm^{-1} and 4315 cm^{-1} given by Walsh and Warsop [13] and from theoretical considerations that at high energies the spacing between the levels should become nearly equal to one-half the (0100) value. Also pertaining to this region are the rotational constants B_4 and C_4 which are taken equal to the averages of the values for $v_2=3^s$ and 3^a. The anharmonicity coefficients x_{12}, x_{13}, x_{14}, x_{23}, x_{24}, x_{33}, and x_{34} are from [4], and the coefficients x_{44} and g_{44} are from [10]. The anharmonicity coefficient x_{11} is estimated from data for similar stretching vibrations. The coupling constants α_i^N are from [4]. The small coefficient g_{33} is taken as zero.

The values used for the atomic masses are from Cameron and Wichers [35]. The values used for the other physical constants are given in [36].

4. Thermodynamic Functions

The thermodynamic properties of ammonia as an ideal gas at a pressure of one atmosphere are listed in table 3. These include the Gibbs (free) energy function, enthalpy function, heat capacity at constant pressure, and entropy tabulated in dimensionless units at closely spaced temperature intervals from 50 to 5000 °K. Should it be desired to obtain the properties for a pressure of 1 bar (10^6 dynes cm^{-2} or 10^5 Nm^{-2}) the magnitude of the tabulated free energy and entropy values should be increased by 0.0132. Conversion factors to other units in frequent use are given in table 4. The entries in table 3 are truncated at four decimals (except for C_p°/R above 2500 °K which is truncated at three) but at best they are accurate to three decimals. It is felt that the additional significance could be useful in applications involving differences between the entries. The density of entries permits use of linear interpolation throughout the table with a resulting interpolation error smaller than the uncertainty in the tabulated values.

As indicated by the earlier discussion the present calculation, except for the out-of-plane vibrations, is based on an expansion about the harmonic oscillator-rigid rotator model. In this expansion only first order (linear) terms in the coupling between the various degrees of freedom are retained. In addition to the errors inherent in the derivation of the partition function, eq (16), there are also errors due to uncertainties in the molecular constants, errors which arise from certain resonances between several of the low-lying vibrational states, the effects of which are omitted, and lastly errors arising from omission of excited electronic states.

TABLE 3. *Thermodynamic functions for ammonia*

The tabulated values are spaced sufficiently close to permit linear interpolation between the entries with a resulting error less than their overall uncertainty. For convenience the values at 273.15 and 298.15 °K have also been included.

T	$(E_0^\circ-G)/RT$	$(H^\circ-E_0^\circ)/RT$	C_p°/R	S°/R
50.	12.0017	3.9539	4.0029	15.9555
60.	12.7234	3.9620	4.0026	16.6854
70.	13.3346	3.9678	4.0026	17.3024
80.	13.8648	3.9721	4.0027	17.8369
90.	14.3328	3.9756	4.0029	18.3084
100.	14.7519	3.9783	4.0033	18.7302
110.	15.1311	3.9806	4.0039	19.1117
120.	15.4776	3.9826	4.0051	19.4602
130.	15.7964	3.9844	4.0069	19.7808
140.	16.0918	3.9861	4.0097	20.0779
150.	16.3668	3.9878	4.0138	20.3546
160.	16.6243	3.9896	4.0194	20.6138
170.	16.8662	3.9915	4.0267	20.8577
180.	17.0944	3.9937	4.0358	21.0881
190.	17.3104	3.9962	4.0468	21.3066
200.	17.5154	3.9991	4.0599	21.5145
210.	17.7106	4.0023	4.0749	21.7129
220.	17.8969	4.0060	4.0920	21.9029
230.	18.0751	4.0101	4.1110	22.0852
240.	18.2458	4.0147	4.1319	22.2606
250.	18.4098	4.0199	4.1548	22.4297
260.	18.5676	4.0255	4.1794	22.5931
270.	18.7196	4.0317	4.2057	22.7513
273.15	18.7663	4.0338	4.2143	22.8001
280.	18.8664	4.0384	4.2336	22.9048
290.	19.0082	4.0456	4.2630	23.0539
298.15	19.1204	4.0520	4.2882	23.1724
300.	19.1455	4.0534	4.2939	23.1989
310.	19.2785	4.0617	4.3260	23.3402
320.	19.4076	4.0704	4.3593	23.4781
330.	19.5330	4.0797	4.3937	23.6127
340.	19.6550	4.0895	4.4291	23.7444
350.	19.7737	4.0997	4.4654	23.8733
360.	19.8893	4.1104	4.5025	23.9997
370.	20.0021	4.1215	4.5402	24.1235

TABLE 3. *Thermodynamic functions for ammonia*—Continued

T	$(E_0^\circ - G)/RT$	$(H^\circ - E_0^\circ)/RT$	C_p°/R	S°/R
380.	20.1121	4.1330	4.5785	24.2451
390.	20.2196	4.1449	4.6173	24.3646
400.	20.3247	4.1572	4.6565	24.4819
410.	20.4275	4.1699	4.6961	24.5974
420.	20.5282	4.1829	4.7359	24.7111
430.	20.6268	4.1962	4.7759	24.8230
440.	20.7234	4.2098	4.8161	24.9332
450.	20.8181	4.2237	4.8563	25.0419
460.	20.9111	4.2379	4.8966	25.1491
470.	21.0024	4.2524	4.9368	25.2548
480.	21.0921	4.2671	4.9771	25.3592
490.	21.1802	4.2820	5.0172	25.4622
500.	21.2669	4.2971	5.0572	25.5640
520.	21.4360	4.3278	5.1368	25.7639
540.	21.6000	4.3593	5.2158	25.9592
560.	21.7591	4.3912	5.2939	26.1503
580.	21.9137	4.4237	5.3712	26.3374
600.	22.0643	4.4566	5.4475	26.5208
620.	22.2109	4.4898	5.5230	26.7007
640.	22.3540	4.5232	5.5975	26.8772
660.	22.4937	4.5569	5.6711	27.0506
680.	22.6302	4.5907	5.7438	27.2210
700.	22.7638	4.6247	5.8157	27.3885
720.	22.8946	4.6588	5.8867	27.5533
740.	23.0227	4.6929	5.9568	27.7156
760.	23.1483	4.7271	6.0261	27.8754
780.	23.2715	4.7613	6.0946	28.0328
800.	23.3925	4.7954	6.1622	28.1879
820.	23.5113	4.8296	6.2291	28.3409
840.	23.6281	4.8637	6.2952	28.4918
860.	23.7430	4.8978	6.3604	28.6407
880.	23.8559	4.9317	6.4249	28.7877
900.	23.9672	4.9656	6.4885	28.9328
920.	24.0767	4.9994	6.5513	29.0761
940.	24.1845	5.0331	6.6133	29.2176
960.	24.2909	5.0667	6.6745	29.3575
980.	24.3957	5.1001	6.7348	29.4958
1000.	24.4990	5.1334	6.7943	29.6324
1020.	24.6010	5.1665	6.8530	29.7676
1040.	24.7017	5.1995	6.9108	29.9012
1060.	24.8010	5.2323	6.9678	30.0334
1080.	24.8991	5.2650	7.0239	30.1641
1100.	24.9960	5.2975	7.0792	30.2935
1120.	25.0918	5.3298	7.1335	30.4216
1140.	25.1864	5.3619	7.1870	30.5483
1160.	25.2799	5.3938	7.2397	30.6738
1180.	25.3724	5.4256	7.2914	30.7980
1200.	25.4639	5.4571	7.3424	30.9209
1220.	25.5543	5.4884	7.3924	31.0427
1240.	25.6438	5.5195	7.4416	31.1633
1260.	25.7324	5.5504	7.4900	31.2828
1280.	25.8200	5.5811	7.5375	31.4011
1300.	25.9068	5.6115	7.5841	31.5183
1320.	25.9927	5.6418	7.6299	31.6345
1340.	26.0778	5.6718	7.6749	31.7495
1360.	26.1620	5.7016	7.7190	31.8636
1380.	26.2455	5.7311	7.7624	31.9766
1400.	26.3281	5.7604	7.8049	32.0886
1420.	26.4101	5.7895	7.8466	32.1996
1440.	26.4912	5.8184	7.8875	32.3096

TABLE 3. *Thermodynamic functions for ammonia*—Continued

T	$(E_0^\circ-G)/RT$	$(H^\circ-E_0^\circ)/RT$	C_p°/R	S°/R
1460.	26.5717	5.8470	7.9277	32.4187
1480.	26.6514	5.8754	7.9671	32.5268
1500.	26.7305	5.9035	8.0058	32.6340
1550.	26.9252	5.9729	8.0992	32.8981
1600.	27.1159	6.0407	8.1881	33.1566
1650.	27.3028	6.1071	8.2728	33.4099
1700.	27.4861	6.1720	8.3532	33.6581
1750.	27.6659	6.2354	8.4298	33.9013
1800.	27.8424	6.2974	8.5027	34.1398
1850.	28.0158	6.3579	8.5719	34.3737
1900.	28.1862	6.4171	8.6378	34.6032
1950.	28.3536	6.4748	8.7004	34.8284
2000.	28.5182	6.5312	8.7599	35.0494
2050.	28.6802	6.5863	8.8164	35.2664
2100.	28.8395	6.6400	8.8702	35.4795
2150.	28.9964	6.6925	8.9214	35.6889
2200.	29.1508	6.7437	8.9701	35.8945
2250.	29.3030	6.7937	9.0162	36.0966
2300.	29.4528	6.8425	9.0602	36.2953
2350.	29.6005	6.8901	9.1021	36.4906
2400.	29.7460	6.9366	9.1418	36.6826
2450.	29.8895	6.9820	9.1797	36.8715
2500.	30.0310	7.0263	9.216	37.0573
2550.	30.1706	7.0696	9.250	37.2402
2600.	30.3083	7.1118	9.282	37.4201
2650.	30.4441	7.1531	9.313	37.5972
2700.	30.5782	7.1933	9.342	37.7716
2750.	30.7106	7.2327	9.370	37.9432
2800.	30.8413	7.2711	9.397	38.1123
2850.	30.9703	7.3086	9.422	38.2789
2900.	31.0977	7.3452	9.445	38.4429
2950.	31.2236	7.3810	9.468	38.6046
3000.	31.3479	7.4160	9.490	38.7639
3100.	31.5922	7.4835	9.529	39.0757
3200.	31.8308	7.5480	9.564	39.3788
3300.	32.0640	7.6096	9.596	39.6736
3400.	32.2921	7.6684	9.623	39.9605
3500.	32.5152	7.7246	9.648	40.2398
3600.	32.7336	7.7783	9.670	40.5119
3700.	32.9474	7.8297	9.688	40.7771
3800.	33.1568	7.8788	9.704	41.0357
3900.	33.3621	7.9258	9.717	41.2879
4000.	33.5633	7.9707	9.728	41.5341
4100.	33.7607	8.0137	9.737	41.7744
4200.	33.9543	8.0548	9.743	42.0091
4300.	34.1443	8.0941	9.748	42.2384
4400.	34.3308	8.1317	9.750	42.4626
4500.	34.5140	8.1677	9.751	42.6817
4600.	34.6939	8.2021	9.749	42.8960
4700.	34.8706	8.2350	9.746	43.1056
4800.	35.0443	8.2664	9.741	43.3107
4900.	35.2151	8.2964	9.734	43.5115
5000.	35.3833	8.3253	9.725	43.7086

The expansion about the harmonic oscillator limit is essentially a low temperature expansion, and the errors resulting therefrom for a particular vibrational mode are small provided $\frac{\nu}{T}$ is large, and are of the order of about the square of the linear term. The

Table 4

Conversion factors to convert tabulated value to quantity having dimensions indicated below	Multiply by
Cal mole^{-1} °K^{-1}	1.98717
Cal g^{-1} °K^{-1}	0.116682
Joules mole^{-1} °K^{-1}	8.3143
Joules g^{-1} °K^{-1}	0.488197

largest error of this type occurs for the ν_4 mode. Thus for the most sensitive function, the heat capacity, the uncertainty at 2000 °K is less than 10^{-2} dimensionless units, but increases to the order of 0.1 at 5000 °K. The higher order anharmonicities would contribute an uncertainty perhaps as large. Though the anharmonicity coefficients x_{11} and x_{13} have large uncertainties, the errors introduced by these are mitigated by the fact that the fundamentals ν_1 and ν_3 are large. A 50 percent uncertainty in x_{11} and x_{13} results in an error of about 0.05 dimensionless units in C_p°/R at 5000 °K. Setting g_{33} equal to zero introduces negligible error since this coefficient introduces a small correction to an already small anharmonic contribution (owing to the large value of the ν_3 fundamental). The remaining anharmonicities (other than the x_{22} value in table 2) are probably accurate to better than several percent, and the uncertainties resulting from these are comparatively small. Uncertainties arising from errors in the rotational fundamentals are also comparatively small, as are uncertainties resulting from the use of estimates for some of the rotational stretching constants. The uncertainties that arise from errors in the rotation-vibration coupling constants are perhaps half as large as those arising from errors in the anharmonicity coefficients.

The uncertainties in the values used for the fundamental frequencies are less than several tenths of a wavenumber, and the uncertainty from this source is negligible. Also negligible are the uncertainties due to errors in the observed overtones of the ν_2 fundamental.

It is somewhat more difficult to determine the uncertainty resulting from estimates used for the molecular constants in the second term in eq (14). The largest uncertainty here arises from possible errors in ν_2' and E_{4^s}. An uncertainty of several percent in these results in an uncertainty in C_p°/R of less than 0.002 dimensionless units at 1000 °K, which increases to a maximum near 2000 °K of less than 0.01 dimensionless units. The errors from estimates of the vibrational coupling constants used in this term are completely negligible below 2000 °K. Even if a 100 percent uncertainty in their contribution is assumed, the resulting uncertainty at 5000 °K still would be less than 0.1 dimensionless units in C_p°/R.

The spectrum of ammonia is further complicated by several large resonances that occur between some of the low lying vibrational bands, such as the resonance between the combination bands $(2\nu_4+\nu_3)$ and $(\nu_1+\nu_3)$ and between the bands $2\nu_4$ and ν_1 as discussed in [4]. Since the resonances tend to displace the respective bands symmetrically about their unperturbed values, it can be shown that the errors are less than the neglected higher order anharmonicities. A similar type of error occurs in the treatment of the coupling of the ν_2 mode with the other modes. The coupling constants as reported are the average of the symmetric and antisymmetric values. Thus the effect of this approximation is to introduce errors similar to those arising from neglect of the resonances discussed above. The treatment of centrifugal distortion, which includes a quadratic term in the temperature, is consistent with the other approximations and the error from this source at 5000 °K is probably less than 0.05 in C_p°/R. At the low temperature end there is a small error arising from the rotational quantum approximation Q_{qr} (eq (17)). At 100 °K this error is less than 10^{-3} in C_p°/R, but is appreciably larger at 50 °K.

Finally, the U.V. absorption spectrum indicates bands extending from ~ 46,000 cm^{-1} to over 100,000 cm^{-1}, as discussed, for example, in [13]. The error from omission of these even at the very highest temperatures considered here is completely negligible. It is felt, therefore, that the uncertainty in the tables in the temperature region 100 to 1000 °K is probably less than 0.003 dimensionless units in C_p°/R. This uncertainty increases to 0.02 at 2000 °K and then increases very rapidly to perhaps 0.3 at 5000 °K. A more complete list of the uncertainty estimates, including those for the enthalpy and entropy, are given in table 5.

Table 5. *Estimates of uncertainty in dimensionless units*

T	$\Delta C_p^\circ/R$	$\Delta(H^\circ-E_0^\circ)/RT$	$\Delta S^\circ/R$
100	0.003	0.002	0.003
1000	.003	.002	.003
2000	.02	.01	.02
3000	.05	.02	.03
4000	.1	.05	.07
5000	.3	.1	.2

5. Discussion

Ideal-gas calculations for NH_3 have been reported in the literature since the early thirties, but many of these calculations were based on relatively incomplete and inaccurate molecular data and on simplified structural models. Also, for the most part, the temperature ranges were somewhat limited. The references [17–27] are representative of these early efforts.

Some of the more recent calculations which have been widely used include those of Harrison and Kobe [28] who calculated the heat capacity, enthalpy, and entropy from 273.16 to 1500 °K. They included the major effects associated with the molecular inversion by summing the lower states of the ν_2 mode term by term, but omitted all vibration and rotational coupling effects other than rotational stretching. The review by Davies reported in the monograph edited by Din [29] includes the specific heat, entropy, and enthalpy from 200 to 1000 °K. The calculation follows essentially the procedure in [28], except that centrifugal stretching is omitted. Also it appears that the contribution of the states in the term-by-term sum of the ν_2 mode was omitted above the level 3^a. The most detailed of the previous calculations is that reported by Yungman et al. [30], (which also appears in [16]), in which the free energy, entropy, and enthalpy are tabulated at 100 °K intervals from 298.15 to 6000 °K. In addition to the term-by-term sum for the ν_2 mode, this work also includes several of the first order vibrational and rotational coupling contributions. It omits, however, the contributions due to coupling of the ν_2 mode with the other vibrational modes, and includes a somewhat simplified coupling of the ν_2 mode with rotation. These calculations are based on essentially the same molecular data as those reported here, except that the values used for the vibrational coupling constants x_{13} and x_{44} are about twice as large. One of the most widely used set of tables is that of JANAF [31]. The reference refers to the latest revision for ammonia, September 30, 1965. This calculation follows the procedures of [28] and [30], though the specific details are not given in the text. Finally, there are several recent calculations based on somewhat simplified molecular models, which are included in references [32–34].

The figures 1 and 2 include a comparison of some of the previous calculations with those made here. The ordinates are the deviations from the present calculations, that is the present calculation minus the others. Figure 1 is a plot of entropy differences, and figure 2 is a plot of heat capacity differences. It is most interesting to compare the data of Yungman et al. [30], curve #5 in figure 1. At the low temperatures the agreement is quite good, but as the temperature is increased, a positive deviation occurs until about 3000 °K, when the deviation becomes strongly negative. The difference at the lower temperatures is probably due to their simplified treatment of the coupling of the ν_2 mode with rotation. At temperatures above 1000 °K, the dominant contribution to the difference is from the x_{24} term omitted in [30] which yields a positive contribution. At temperatures above 3000 °K, the dominant contribution is from the omitted x_{12} and x_{23} terms which yield large negative contributions. In addition to these, the high value they used for x_{44} (larger by a factor of two) tends to reduce the differences at temperatures below 3000 °K, but magnifies them above. The same general comments apply to the JANAF [31] comparison as seen in curve #1, except that the difference goes negative at somewhat higher temperatures and the positive deviations are considerably larger. Incidentally, the JANAF and Harrison and Kobe [28] (curve #4) calculations are nearly identical for temperatures up to 1000 °K. Curve #3 applies to a modified rigid rotator harmonic oscillator calculation as given in an older (now superseded) JANAF table. The comparison for curve #2 [29] illustrates the sensitivity to the omission of the hierarchy of states corresponding to large v_2 quantum numbers ($v_2 > 3$). The differences plotted in figure 2 exhibit essentially the same behavior as those in figure 1 except that they are somewhat larger.

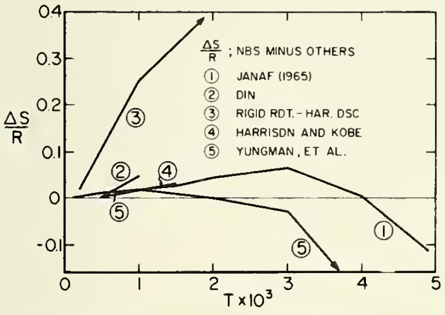

FIGURE 1. *Dimensionless entropy differences.*

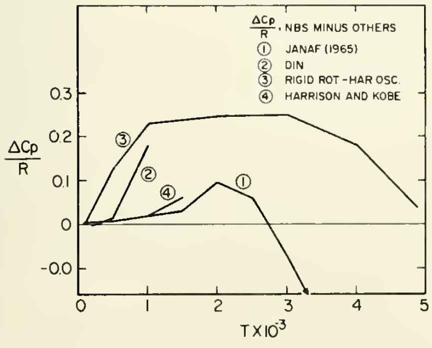

FIGURE 2. *Dimensionless heat capacity differences.*

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