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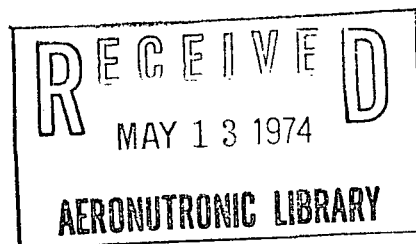
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**TRANSPORT PROPERTIES OF N₂ GAS
AT CRYOGENIC TEMPERATURES**

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TRANSPORT PROPERTIES OF N₂ GAS AT CRYOGENIC TEMPERATURES

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SUMMARY

The viscosity and thermal conductivity of nitrogen gas for the temperature range 5° K - 135° K have been computed from the second Chapman-Enskog approximation. Quantum effects, which become appreciable at the lower temperatures, are included by utilizing collision integrals based on quantum theory. A Lennard-Jones (12-6) potential was assumed. The computations yield viscosities about 20 percent lower than those predicted for the high end of this temperature range by the method of corresponding states, but the agreement is excellent when the computed values are compared with existing experimental data.

INTRODUCTION

Considerable interest has developed in the design of a nitrogen wind tunnel to operate at cryogenic temperatures. Such a facility permits flow with a very high Reynolds number ($Re = \rho v l / \eta$), because the viscosity η is small at low temperatures. However, gases at cryogenic temperatures exhibit anomalous properties, and the designer is immediately faced with the problem of accurately determining the viscosity in the presence of these so-called "quantum effects."

Two kinds of quantum phenomena affect the transport properties of gases at low temperatures (ref. 1). Diffraction effects, which result from the wave nature of molecules, and symmetry effects, which are a consequence of the Pauli exclusion principle, increase as the deBroglie wavelength becomes large. For diffraction effects to become important, the deBroglie wavelength λ_0 must enlarge to the order of molecular dimensions. Symmetry effects are not sizable until λ_0 has increased to the order of the distance between molecules. For a molecule with arithmetic mean velocity at temperature T ,

$$\lambda_0 = \frac{27.4 \text{ \AA}}{\sqrt{MT}}$$

where M is the molecular weight, and T is the temperature in degrees Kelvin. This simple relationship shows that above 200° K, quantum effects are negligible, even for lighter gases; however, under 100° K, the transport properties can be in serious error if quantum effects are neglected.

The equilibrium separation of the two atomic nuclei in a ground state N₂ molecule is about 1.05 Å. If this molecule has arithmetic mean velocity

at 80° K, its deBroglie wavelength is about 0.6 Å, and diffraction has begun to influence the transport properties. Symmetry effects, however, will not become important except at very high densities or until the temperature has dropped to below 2° K.

Two methods have long been used for predicting transport properties of gases; one is based on the principle of corresponding states and the other on Chapman-Enskog theory. The method of corresponding states is semi-empirical and works best for dense gases and higher temperatures (ref. 2), while Chapman-Enskog theory is applicable for dilute gases (ref. 1). Since there is no lack of experimental data at temperatures over 100° K and since the application of Chapman-Enskog theory requires long and tedious calculations, the method of corresponding states has been the most useful in predicting transport properties. At low temperatures, however, there is a paucity of experimental data, gases must necessarily be dilute to remain gaseous, and Chapman-Enskog theory must be used. In this paper, the Chapman-Enskog theory is used to calculate the transport properties of nitrogen in the temperature range 5°-135° K with quantum effects included.

THEORETICAL BACKGROUND

Chapman-Enskog theory gives the transport coefficients of a dilute gas in terms of collision integrals $\Omega^{(\ell, s)}(T)$. Although these integrals are functions of the temperature T , their calculation involves the dynamics of a molecular encounter, and hence they depend on the intermolecular potential. More complicated potential forms have been proposed to empirically fit viscosity data over a wide range of temperatures (ref. 3), but the Lennard-Jones potential $\phi(r) = 4\epsilon\{(\sigma/r)^{12} - (\sigma/r)^6\}$ has been most widely used. The constants σ and ϵ are the zero crossing and the well depth, respectively. The numerical values used for N₂ in this paper are $\epsilon/k = 91.5^\circ$ K, where k is Boltzmann's constant and $\sigma = 3.681$ Å. These values were determined by Johnston and McCloskey (ref. 4) from viscosity data taken in the range 80° K $\leq T \leq 300^\circ$ K.

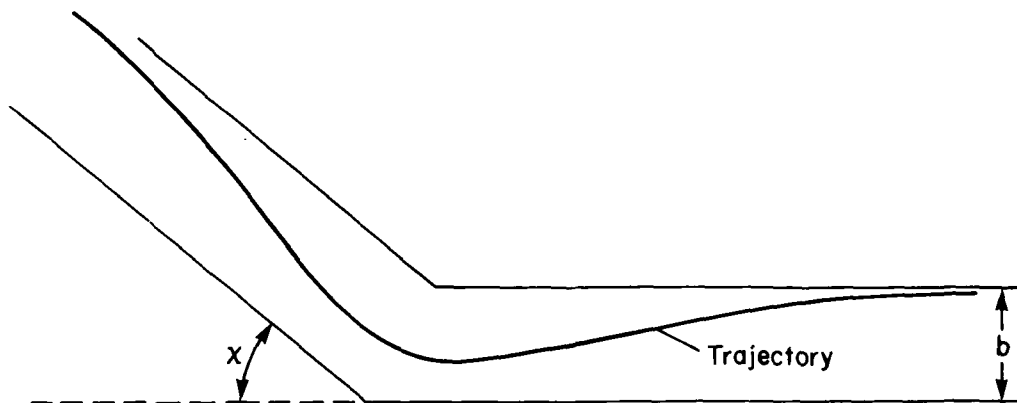
The collision integrals take the form

$$\Omega^{(\ell, s)}(T) = \left(\frac{kT}{2\pi\mu}\right)^{1/2} \int_0^\infty x^{2s+3} e^{-x^2} S^{(\ell)}(kTx) dx \quad (1)$$

in which μ is the reduced mass of the collision partners and $S^{(\ell)}(E)$ is the collision cross section ($E = \mu V_0^2/2$ where V_0 is the initial relative velocity of the colliding molecules). The dimensionless collision energy x is defined by $x = E/kT$. For high-energy collisions, the trajectory of the collision partners is assumed to be classical and the cross section is given by

$$S^{(\ell)}(E) = 2\pi \int_0^\infty b(1 - \cos^\ell \chi) db \quad (2)$$

where b is the impact parameter and χ is the classical angle of deflection in the center mass coordinates as shown in sketch (a).



Sketch (a)

The deflection angle and the intermolecular potential are related by

$$\chi = \pi - 2b \int_{r_m}^{\infty} \frac{dr}{r^2 f(r)} \quad (3)$$

where the classical turning point r_m is the outermost zero of

$$f(r) = \sqrt{1 - \frac{\phi(r)}{E} - \frac{b^2}{r^2}}$$

When the classical approximation is permissible, the problem of calculating the collision integrals $\Omega^{(l,s)}(T)$ reduces to a numerical triple integration via equations (1), (2), and (3). Although the calculation is itself difficult, tables of classical collision integrals for simple interaction potentials have been available for many years (refs. 1,5). If quantum effects are to be included in calculating the collision integrals, the classical cross section must be replaced by a quantal cross section. This step complicates the computational problem so much that, until recently, it has been prohibitive.

In the quantum theory, it is not possible to define an exact angle of deflection because the position and velocity vector of the molecule cannot be simultaneously known. It is only possible to give a probability for the deflection angle χ . The expression for the quantal cross section is

$$S^{(l)}(E) = 2\pi \int_0^{\pi} |f(\chi)|^2 (1 - \cos^l \chi) \sin \chi d\chi \quad (4)$$

where $|f(\chi)|^2$ is the probability of a deflection χ , and the function $f(\chi)$ is called the scattering amplitude.

$$f(\chi) = \frac{\hbar}{2i\sqrt{2\mu E}} \sum_{n=0}^{\infty} (2n+1) P_n(\cos \chi) \{e^{2i\delta_n} - 1\} \quad (5)$$

In equation (5), n is the angular momentum quantum number and δ_n is the phase shift induced in the radial wave function of a pair with angular momentum $\hbar\sqrt{n(n+1)}$ by their collision. (In a classical sense, this angular momentum is μbV_0 .)

Expressions for the viscosity and thermal conductivity of nitrogen involve the integrals $\Omega^{(2,2)}$ and $\Omega^{(2,3)}$, and these require only the cross section $S^{(2)}(E)$. It has been found (ref. 1) that when equation (5) is inserted into equation (4), $S^{(2)}(E)$ simplifies to

$$S^{(2)}(E) = \frac{4\pi\hbar^2}{2\mu E} \sum_n \frac{(n+1)(n+2)}{(2n+3)} \sin^2(\delta_n - \delta_{n+2})$$

At low temperatures, the angular momentum must be at or near the angular momentum ground state $n=0$, so that only a few terms in this summation contribute.

Rigorous evaluation of the quantal phase shifts δ_n requires numerical solutions of the Schrödinger wave equation, and this is a very difficult numerical problem in itself. As a result, the semiclassical *JWKB* approximation (ref. 6), has been widely used:

$$\delta_n(JWKB) = \frac{\hbar}{\sqrt{2\mu E}} \lim_{R \rightarrow \infty} \left\{ \int_{r_m}^R \left[1 - \frac{\phi(r)}{E} - \frac{p^2}{r^2} \right]^{1/2} dr - \int_b^R \left[1 - \frac{p^2}{r^2} \right]^{1/2} dr \right\} \quad (6)$$

in which $p = [(n+1/2)\sqrt{2\mu E}]/\hbar$. However, a critical study of the use of this approximation (ref. 7) has shown it to be unsatisfactory except in a limited region of high values for E and low values for the deBroglie wavelength. It is not a practical tool at low temperatures, where exact quantal phase shifts are required if quantum effects are to be included in the collision integrals. The availability of high-speed computing machines has made the numerical solution of Schrödinger's equation practicable, even for a large number of combinations of b , E , σ , and ϵ , and efficient numerical methods have been developed to compute the δ_n with accuracy (ref. 7).

CALCULATIONS AND COMPARISONS

The transport properties are most conveniently expressed in terms of reduced collision integrals $\Omega^{(\ell, s)*}(T^*)$.

$$\Omega(i, j)^*(T^*) = [(j + 1)!(T^*)^{j+2}]^{-1} \int_0^\infty \exp \left\{ -\frac{E^*}{T^*} \right\} E^{*(j+1)} S(i)^*(E^*) dE^* \quad (7)$$

where $T^* = kT/\epsilon$, $E^* = (1/2\epsilon)\mu V_0^2$, and $S(i)^*(E^*)$ is the usual reduced collision cross section (e.g., $S(1)^* = S(1)/\pi\sigma^2$). The viscosity η and thermal conductivity λ are then given by

$$\frac{\eta}{[\eta]_1} = 1 + \frac{3}{196} \left[\frac{8\Omega(2,3)^*}{\Omega(2,2)^*} - 7 \right]^2 + \dots \quad (8)$$

$$\frac{\lambda}{[\lambda]_1} = 1 + \frac{1}{42} \left[\frac{8\Omega(2,3)^*}{\Omega(2,2)^*} - 7 \right]^2 + \dots \quad (9)$$

In these equations, $[\eta]_1$ and $[\lambda]_1$ are the first-order Chapman-Enskog approximations. If M is the molecular weight of the gas, and σ is given in Å,

$$[\eta]_1 = 10^{-7} \times \frac{266.93\sqrt{MT}}{\sigma^2 \Omega(2,2)^*(T^*)} \quad \text{poise} \left(\frac{\text{dyne}}{\text{cm}^2 \text{sec}^{-1}} \right)$$

$$[\lambda]_1 = 10^{-7} \times \frac{1989.1}{\sigma^2 \sqrt{M}} \cdot \frac{\sqrt{T}}{\Omega(2,2)^*(T^*)} \quad \frac{\text{cal}}{\text{cm-sec}^\circ \text{K}}$$

Tables (ref. 8) of the reduced collision integrals, based on exact quantal phase shifts, have been calculated (ref. 9) for the Lennard-Jones potential.

Since $\Omega(i, j)^*(T^*)$ is a function of the intermolecular potential as well as T^* , the collision integrals are given for the temperature range $0.01^\circ \text{K} \leq T^* \leq 100^\circ \text{K}$ and several values of the reduced deBroglie wavelength $\Lambda^* = h/\sigma\sqrt{2\mu\epsilon}$. This parameter is a measure of the quantum nature of the gas at a given temperature, and $\Lambda^* \rightarrow 0$ as the gas becomes more nearly "classical." For He, $\Lambda^* = 2.67$, but for the heavier N_2 , it is about an order of magnitude smaller. In the tables, Λ^* increases from $\Lambda^* = 0$ to $\Lambda^* = 3.5$ in increments of 0.5.

The collision integrals used to calculate the transport properties of N_2 ($\Lambda^* = 0.229$) were obtained by interpolation in the tables. These interpolated values are listed as a function of T^* in table 1, which also gives the viscosity and thermal conductivity computed from equations (8) and (9). Figure 1 compares the numerical values for viscosity from table 1 with the existing experimental values (refs. 4,10) and the values predicted by the method of corresponding states (ref. 11). The excellent agreement with experiment at the high end of the temperature range gives credibility to the calculated viscosity at lower temperatures. Experimental data are not available for temperatures below 78.6°K . While the method of corresponding

states gives a viscosity that is about 20 percent too high at 78.6° K, it predicts with better accuracy at temperatures above 150° K.

The thermal conductivity for N₂ is plotted in figure 2.

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National Aeronautics and Space Administration
Moffett Field, Calif. 94035, January 23, 1974

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TABLE 1.— COLLISION INTEGRALS, VISCOSITY, AND THERMAL
CONDUCTIVITY FOR N₂

$T(^{\circ}\text{K})$	$T^* = \frac{kT}{\epsilon}$	$\Omega(2,2)^*$	$\Omega(2,3)^*$	$\eta(\text{micropoise})$	$\lambda\left(\frac{\text{microcal}}{\text{cm sec } ^{\circ}\text{K}}\right)$
4.575	0.05	5.36094	4.91758	4.16639	1.10990
5.49	0.06	5.03710	4.59643	4.85525	1.29307
6.405	0.07	4.75956	4.30643	5.54773	1.47715
7.320	0.08	4.51737	4.06478	6.24722	1.63156
8.235	0.09	4.30615	3.86419	6.95025	1.85020
9.15	0.10	4.12353	3.70038	7.65067	2.03666
13.725	0.15	3.53156	3.23046	10.95231	2.91729
18.3	0.20	3.22622	2.98744	13.85738	3.69313
22.875	0.25	3.01906	2.78798	16.55204	4.41068
27.45	0.30	2.84634	2.60182	19.21670	5.11847
32.025	0.35	2.69056	2.42970	21.9423	5.84208
36.60	0.40	2.54776	2.27453	24.7606	6.59077
41.175	0.45	2.41723	2.13711	27.67445	7.36545
45.75	0.50	2.29863	2.01660	30.67422	8.16348
54.9	0.60	2.09469	1.81955	36.8747	9.81383
64.05	0.70	1.92925	1.66961	43.2469	11.51005
82.35	0.90	1.68493	1.46096	56.14634	14.94298
91.5	1.00	1.59421	1.39776	62.54767	16.64610
137.25	1.50	1.31406	1.17349	92.96598	24.74580

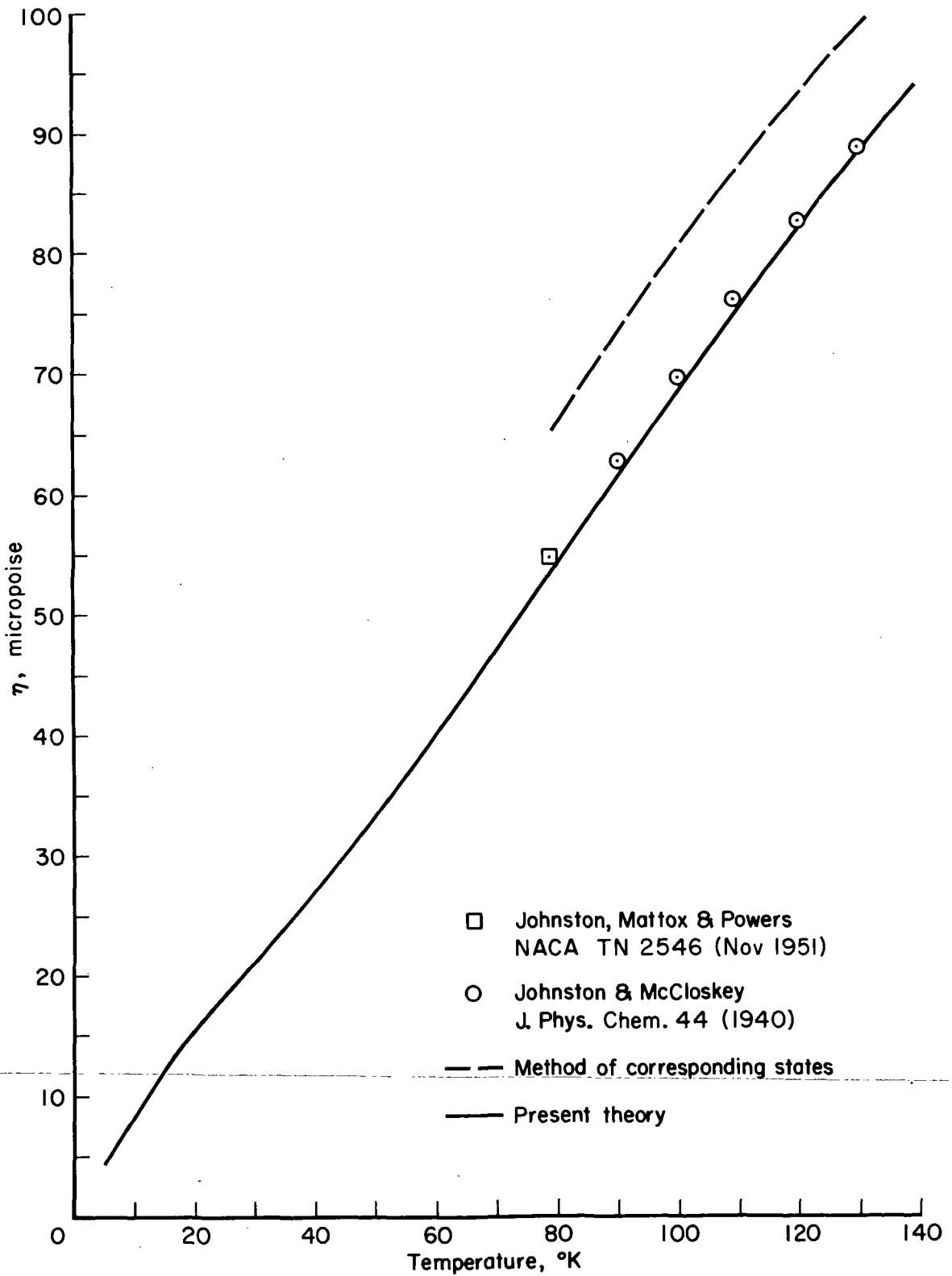


Figure 1.— Calculated and experimental viscosity of N₂.

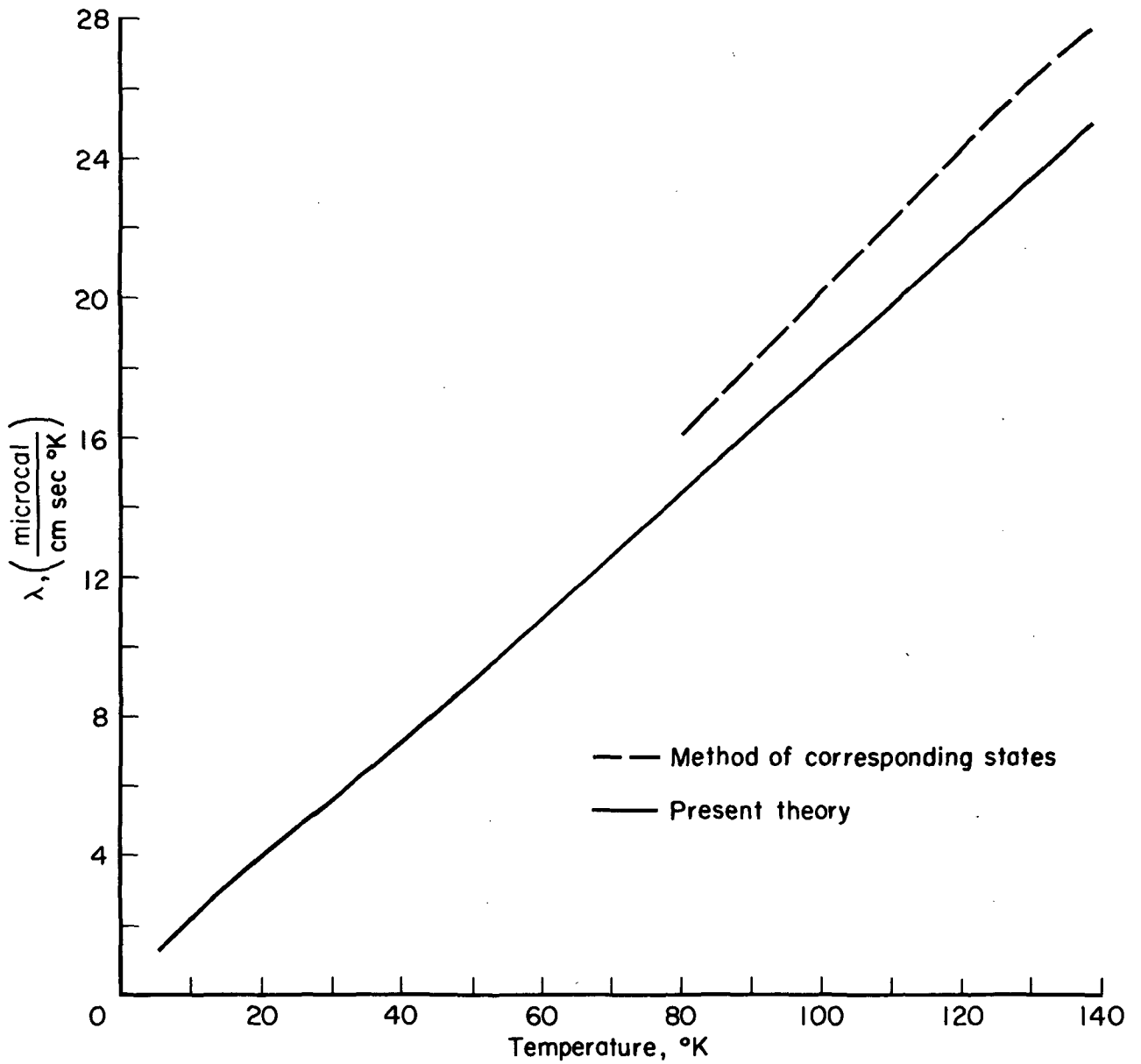
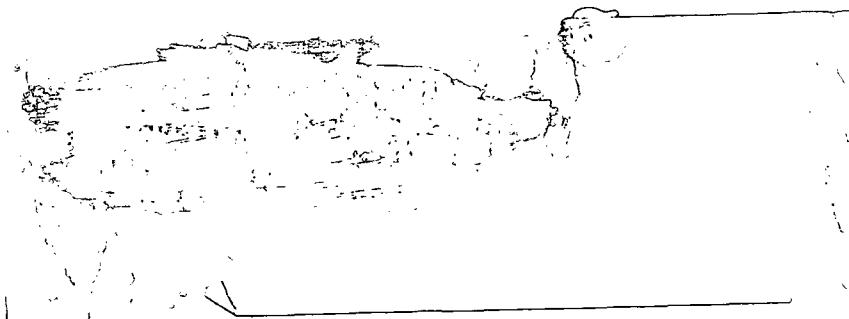


Figure 2.— Calculated thermal conductivity of N_2 .



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