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PUBCO-I, AN IBM 704 CODE
FOR COMPUTING THE IDEAL THERMODYNAMIC FUNCTIONS
OF A POLYATOMIC GAS MOLECULE

LOS ALAMOS NATIONAL LABORATORY



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LOS ALAMOS SCIENTIFIC LABORATORY
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PUBCO-I, AN IBM 704 CODE
FOR COMPUTING THE IDEAL THERMODYNAMIC FUNCTIONS
OF A POLYATOMIC GAS MOLECULE

by

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ABSTRACT

The PUBCO-I code computes the ideal thermodynamic functions of polyatomic molecules by either the rigid rotator-harmonic oscillator (RRHO) or the non-rigid rotator-anharmonic oscillator (NRRAO) method. The type of computation performed by the IBM 704 is at the option of the operator and will depend, in general, upon the availability of sufficient spectroscopic data to carry out the NRRAO calculations.

The equations used to describe the thermodynamic functions in the two treatments are discussed. A general description of the code is presented and the complete IBM listing for the code is given. Sample computations of the ideal thermodynamic functions of HCN are given for both the RRHO molecule and the NRRAO molecule.

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1. INTRODUCTION

The prediction of chemical reactions by means of the free energy functions of the participating chemical species enables one to concentrate his effort upon those processes which are fruitful and to bypass those which would lead into blind alleys. The generation of thermodynamic data can be accomplished rather effortlessly by the use of modern electronic computing machines if the general codes to perform the calculations are available. This report describes one such code, PUBCO-I, which will perform these calculations for polyatomic molecules on an IBM 704 electronic computer.

The code consists of two sections; the first computes the ideal thermodynamic functions for a rigid rotator-harmonic oscillator (RRHO) molecule, and the second computes the necessary corrections to the ideal thermodynamic functions due to the nonrigid rotation and anharmonicity of the molecule. The computation of the correction terms is performed at the option of the operator and, in general, is limited by the availability of sufficient spectroscopic data to permit this phase of the calculation to be carried out.

The equations which are used in the computation of the thermodynamic functions by means of the PUBCO-I code are discussed in Section 2; a general description of the code is given in Section 3; the IBM listing for the code is reproduced in Appendix A; and sample machine printouts for HCN, both RRHO and NRRAO, are given in Appendix B and Appendix C, respectively.

2. THERMODYNAMIC FUNCTIONS OF POLYATOMIC MOLECULES

2.1 Partition Functions

The thermodynamic functions of any gaseous molecule can be computed by means of the partition function^{1,2} defined as

$$Q = \sum_i g_i e^{-\epsilon_i/kT}, \quad (1)$$

where

g_i = degeneracy of the i th energy level,

ϵ_i = energy of the i th energy level,

k = Boltzmann constant,

T = absolute temperature in degrees Kelvin.

It is possible to factor the total partition function, Q , into an internal and a translational partition function such that

$$Q = Q_{\text{int}} \cdot Q_{\text{tr}}. \quad (2)$$

Moreover, if the various possible interactions are neglected, the internal partition function is separable into an electronic component, a vibrational component, and a rotational component with the result that

$$Q = Q_{\text{tr}} \cdot Q_{\text{el}} \cdot Q_{\text{vib}} \cdot Q_{\text{rot}}. \quad (3)$$

It can be shown that the translational partition function, Q_{tr} , can be expressed as

$$Q_{\text{tr}} = V \left(\frac{2\pi mkT}{h^2} \right)^{3/2}, \quad (4)$$

where

V = volume of gas being considered,

m = absolute mass of the molecule,

h = Planck constant.

The electronic partition function, Q_{el} , is defined as

$$Q_{el} = g_{el} e^{-\epsilon_{el}/kT}, \quad (5)$$

where

g_{el} = degeneracy of the electronic state,

ϵ_{el} = energy of the electronic state.

For all polyatomic molecules except those with unpaired electrons (free radicals), the electronic degeneracy is equal to unity. The ground electronic state has zero energy so that, in general,

$$Q_{el} = 1. \quad (6)$$

The vibrational partition function for a harmonic oscillator can be expressed as

$$Q_{vib} = \sum_{v=0}^{\infty} g_v e^{-(hcv/kT)(\omega_1 + \omega_2 + \dots)} \quad (7)$$

$$Q_{vib} = \prod_i \left(\sum_{v=0}^{\infty} g_i e^{-hcv\omega_i/kT} \right) \left(\sum_{v=0}^{\infty} g_2 e^{-hcv\omega_2/kT} \right) \dots, \quad (8)$$

where

g_i = degeneracy of i th vibrational level,

c = velocity of light,

v = vibrational quantum number = 0, 1, 2, . . . ,

ω_i = i th fundamental vibrational frequency (cm^{-1}).

Each of the sums in the vibrational partition function can be simplified to

$$\sum_{v=0}^{\infty} g_i e^{-hcv\omega_i/kT} = g_i \left(1 - e^{-hc\omega_i/kT} \right)^{-1}, \quad (9)$$

so that

$$Q_{vib} = \prod_i g_i \left(1 - e^{-hc\omega_i/kT} \right)^{-1} \quad (10)$$

The vibrational degeneracies, g_i , will cause each degenerate frequency, ω_i , to be considered g_i times in the product (10). In general, in molecular spectra nomenclature, the fundamental frequencies, ω_i , are replaced by the wave numbers, ν_i , of the fundamental vibrational bands.

The rotational partition function, Q_{rot} , assumes different forms for linear and nonlinear molecules. For a linear molecule it can be expressed as

$$Q_{rot} = \sum_{J=0}^{\infty} (2J + 1) e^{-BJ(J+1)hc/kT}, \quad (11)$$

where

J = rotational quantum number = 0, 1, 2, . . . ,

B = rotational constant of the molecule (cm^{-1}).

Equation (11) can be expanded asymptotically to give

$$Q_{rot} = \frac{1}{\sigma} \left[\left(\frac{kT}{hcB} \right) + \frac{1}{3} + \frac{1}{15} \left(\frac{hcB}{kT} \right) + \frac{4}{315} \left(\frac{hcB}{kT} \right)^2 + \frac{1}{315} \left(\frac{hcB}{kT} \right)^3 + \dots \right], \quad (12)$$

where σ is the symmetry number.

The rotational partition function for nonlinear symmetric top molecules is given as

$$Q_{\text{rot}} = \sum_{J=0}^{\infty} \sum_{K=-J}^{+J} (2J + 1) \exp - \left\{ [BJ(J + 1) + (A - B)K^2] \frac{hc}{kT} \right\}, \quad (13)$$

where

A = a rotational constant of molecule (cm^{-1}),

K = angular momentum quantum number.

If the temperature is not extremely low, equation (13) can be replaced by the expression

$$Q_{\text{rot}} = \frac{1}{\sigma} \left\{ e^{Bhc/4kT} \left[\frac{\pi}{B^2 A} \left(\frac{kT}{hc} \right)^3 \right]^{1/2} \left[1 + \frac{1}{12} \left(1 - \frac{B}{A} \right) \left(\frac{Bhc}{kT} \right) + \frac{7}{480} \left(1 - \frac{B}{A} \right)^2 \left(\frac{Bhc}{kT} \right)^2 + \dots \right] \right\}. \quad (14)$$

For spherical top molecules one lets $B = A$. For asymmetric top molecules with rotational constants B and C not too different from one another, one can replace B by $\sqrt{BC}$ in equation (14) to obtain

$$Q_{\text{rot}} = \frac{1}{\sigma} \left\{ e^{\sqrt{BC} hc/4kT} \left[\frac{\pi}{ABC} \left(\frac{kT}{hc} \right)^3 \right]^{1/2} \left[1 + \frac{1}{12} \left(1 - \frac{\sqrt{BC}}{A} \right) \left(\frac{\sqrt{BC} hc}{kT} \right) + \frac{7}{480} \left(1 - \frac{\sqrt{BC}}{A} \right)^2 \left(\frac{\sqrt{BC} hc}{kT} \right)^2 \right] \right\}. \quad (15)$$

The nonrigid rotator-anharmonic oscillator molecules are treated as rigid rotator-harmonic oscillator molecules with three correction terms³ to take care of the stretching, anharmonicity, and vibration-rotation interaction of the molecules.

The partition function for stretching is expressed as

$$Q_{\text{st}} = 1 + \rho T, \quad (16)$$

where

$$\rho = 2 \text{ kD}/\text{hcB}^2. \quad (17)$$

In expression (17) D is the centrifugal distortion constant of the molecule.

The anharmonicity partition function is

$$Q_{\text{anh}} = \prod_{i \leq j} \left[1 + \frac{g_i (g_j + \delta_{ij}) X_{ij} (hc/kT)}{\left(e^{\frac{hc \nu_i}{kT}} - 1 \right) \left(e^{\frac{hc \nu_j}{kT}} - 1 \right)} \right], \quad (18)$$

where

$$\begin{aligned} g_i, g_j &= \text{vibrational degeneracies of } i\text{th and } j\text{th vibrational states,} \\ \delta_{ij} &= \text{Kronecker delta,} \\ X_{ij} &= \text{first anharmonicity constant (cm}^{-1}\text{).} \end{aligned}$$

If a particular X_{ii} is associated with a doubly degenerate vibration, ω_i , it must be replaced^{4,5} by

$$X'_{ii} = X_{ii} + \frac{g_{ii}}{3}, \quad (19)$$

where g_{ii} is the anharmonicity constant (cm^{-1}).

It is convenient to make the replacement

$$u_i = hc\nu_i/kT. \quad (20)$$

The vibration-rotation interaction partition function is expressed as

$$Q_{\text{v-r}} = \prod_i \left[1 + \frac{g_i \delta_i}{\left(e^{u_i} - 1 \right)} \right], \quad (21)$$

where δ_i is the vibration-rotation interaction constant (dimensionless).

2.2 Rigid Rotator-Harmonic Oscillator Thermodynamic Functions

The four thermodynamic functions are derivable from the partition function by means of the following expressions:

Free energy function

$$-(F^\circ - H_0^\circ)/T = R \ln Q \quad (22)$$

Enthalpy function

$$(H^\circ - H_0^\circ)/T = RT \frac{d(\ln Q)}{dT} \quad (23)$$

Entropy

$$S^\circ = (H^\circ - H_0^\circ)/T - (F^\circ - H_0^\circ)/T \quad (24)$$

Heat capacity

$$C_p^\circ = R \frac{d}{dT} \left[T^2 \frac{d(\ln Q)}{dT} \right] \quad (25)$$

Since the entropy is merely the sum of the free energy function and the enthalpy function, it is left to the reader to obtain the actual expression for the entropy contributions of various modes of freedom; only the expressions for the free energy function, the enthalpy function, and heat capacity will be given for RRHO and NRRAO molecules.

Expressions (22), (23), and (25) take the following forms when the total partition function Q is separated into its translational plus electronic component and its remaining internal components:

$$-(F^\circ - H_0^\circ)/T = R \left\{ \frac{5}{2} \ln T + \frac{3}{2} \ln M + 20.1976 - \ln P + \ln g_{el} + \ln Q_{int} \right\}, \quad (26)$$

$$(H^\circ - H_0^\circ)/T = R \left\{ \frac{5}{2} + T \frac{d(\ln Q_{int})}{dT} \right\}, \quad (27)$$

$$C_p^\circ = R \left\{ \frac{5}{2} + \frac{d}{dT} \left[T^2 \frac{d(\ln Q_{\text{int}})}{dT} \right] \right\}. \quad (28)$$

Since only the ground electronic state is considered in the PUBCO-I code, it is permissible to make the following substitution:

$$\ln Q_{\text{int}} = \ln(Q_{\text{vib}} \cdot Q_{\text{rot}}) = \ln Q_{\text{vib}} + \ln Q_{\text{rot}}. \quad (29)$$

The vibrational contributions to the above thermodynamic functions are

$$-(F^\circ - H_0^\circ)/T = R \sum_{i=0}^{\infty} \left[\ln g_i \left(1 - e^{-u_i} \right)^{-1} \right], \quad (30)$$

$$(H^\circ - H_0^\circ)/T = R \cdot \frac{hc}{kT} \sum_{i=0}^{\infty} \left[\frac{g_i \nu_i e^{-u_i}}{\left(1 - e^{-u_i} \right)} \right], \quad (31)$$

$$C_p^\circ = R \cdot \left(\frac{hc}{kT} \right)^2 \sum_{i=0}^{\infty} \frac{g_i \nu_i^2 e^{-u_i}}{\left(1 - e^{-u_i} \right)^2} \quad (32)$$

The rotational contributions to the thermodynamic functions for linear molecules are

$$-(F^\circ - H_0^\circ)/T = R \ln \left\{ \frac{1}{\sigma} \left[\left(\frac{kT}{hcB} \right) + \frac{1}{3} + \frac{1}{15} \left(\frac{hcB}{kT} \right) + \frac{4}{315} \left(\frac{hcB}{kT} \right)^2 + \frac{1}{315} \left(\frac{hcB}{kT} \right)^3 \right] \right\}, \quad (33)$$

$$(H - H_0^\circ)/T = R \left[1 - \frac{1}{3} \left(\frac{hcB}{kT} \right) - \frac{1}{9} \left(\frac{hcB}{kT} \right)^2 - \frac{2.67}{63} \left(\frac{hcB}{kT} \right)^3 \right], \quad (34)$$

$$C_p^\circ = R \left[1 + \frac{1}{9} \left(\frac{hcB}{kT} \right)^2 + \frac{5.34}{63} \left(\frac{hcB}{kT} \right)^3 \right], \quad (35)$$

while for nonlinear molecules they become

$$-(F^\circ - H_0^\circ)/T = \frac{R}{\sigma} \left\{ e^{\sqrt{BC} hc/4kT} \left[\frac{\pi}{ABC} \left(\frac{kT}{hc} \right)^3 \right]^{1/2} \left[1 + \frac{1}{12} \left(1 - \frac{\sqrt{BC}}{A} \right) \left(\frac{\sqrt{BC} hc}{kT} \right) + \frac{7}{480} \left(1 - \frac{\sqrt{BC}}{A} \right)^2 \left(\frac{\sqrt{BC} hc}{kT} \right)^2 \right] \right\}, \quad (36)$$

$$(H^\circ - H_0^\circ)/T = R \left\{ \frac{3}{2} - \left[\left\langle \frac{1}{12} \left(1 - \frac{\sqrt{BC}}{A} \right) + \frac{1}{4} \right\rangle \left(\frac{\sqrt{BC} hc}{kT} \right) - \frac{16}{3} \left(1 - \frac{\sqrt{BC}}{A} \right)^2 \left(\frac{\sqrt{BC} hc}{kT} \right)^2 \right] \right\}, \quad (37)$$

$$C_p^\circ = R \left\{ \frac{3}{2} + \frac{16}{720} \left(1 - \frac{\sqrt{BC}}{A} \right)^2 \left(\frac{\sqrt{BC} hc}{kT} \right)^2 \right\}. \quad (38)$$

2.3 Nonrigid Rotator-Anharmonic Oscillator Thermodynamic Functions

The stretching of a molecule makes the following contributions to the thermodynamic functions:

$$-(F^\circ - H_0^\circ)/T = R \ln(1 + \rho T), \quad (39)$$

$$(H^\circ - H_0^\circ)/T = \frac{R\rho T}{(1 + \rho T)}, \quad (40)$$

$$C_p^\circ = R \left\{ \frac{2\rho T(1 + \rho T) - \rho^2 T^2}{(1 + \rho T)^2} \right\}. \quad (41)$$

The anharmonicity corrections increase the thermodynamic functions by

$$-(F^\circ - H_0^\circ)/T = R \ln \prod_{i \leq j} \left[1 + \frac{g_i (g_j + \delta_{ij}) X_{ij} \frac{hc}{kT}}{(e^{u_i} - 1)(e^{u_j} - 1)} \right], \quad (42)$$

$$(H^\circ - H_0^\circ)/T = -\frac{R}{T} \prod_{i \leq j} \left(\frac{AB' - BA'}{A^2 + AB} \right), \quad (43)$$

$$C_p^\circ = \frac{R}{A^2 T^2} \left\{ \frac{2(BA'^2 - AA'B') - ABA''}{(A + B)} - \left(\frac{AB' - BA'}{A + B} \right)^2 \right\}. \quad (44)$$

In expressions (43) and (44) the following substitutions were made for the purpose of simplification:

$$A = \left(e^{u_i} - 1 \right) \left(e^{u_j} - 1 \right), \quad (45)$$

$$A' = \frac{hc}{k} \left\{ \left(\nu_i + \nu_j \right) e^{(u_i + u_j)} - \nu_i \left(e^{u_i} - 1 \right) - \nu_j \left(e^{u_j} - 1 \right) \right\}, \quad (46)$$

$$A'' = \left(\frac{hc}{k} \right)^2 \left\{ \left(\nu_i + \nu_j \right)^2 e^{(u_i + u_j)} - \nu_i^2 \left(e^{u_i} - 1 \right) - \nu_j^2 \left(e^{u_j} - 1 \right) \right\}, \quad (47)$$

$$B = g_i \left(g_j + \delta_{ij} \right) X_{ij} \frac{hc}{kT}, \quad (48)$$

$$B' = g_i \left(g_j + \delta_{ij} \right) X_{ij} \frac{hc}{k}, \quad (49)$$

$$B'' = 0. \quad (50)$$

The primed functions of A and B are derivatives of A and B taken with respect to $1/T$.

The vibration-rotation interaction term makes the following contributions to the thermodynamic functions:

$$-(F^\circ - H_0^\circ)/T = R \ln \prod_i \left[1 + \frac{g_i \delta_i}{\left(e^{u_i} - 1 \right)} \right], \quad (51)$$

$$(H^\circ - H_0^\circ)/T = \frac{R}{T} \prod_i \left[\frac{g_i \delta_i u_i^T e^{u_i}}{(e^{u_i} - 1)(e^{u_i} - 1 + g_i \delta_i)} \right], \quad (52)$$

$$C_p^\circ = \frac{R}{T^2} \prod_i \left\{ \frac{\left(2g_i \delta_i u_i^T e^{u_i} \right) (e^{u_i} - 1) e^{u_i} u_i T - (e^{u_i} - 1)^2 g_i \delta_i e^{u_i} (u_i T)^2}{(e^{u_i} - 1 + g_i \delta_i) (e^{u_i} - 1)^3} - \left[\frac{g_i \delta_i e^{u_i} u_i T}{(e^{u_i} - 1)(e^{u_i} - 1 + g_i \delta_i)} \right]^2 \right\}. \quad (53)$$

Summation of all the contributions to any particular thermodynamic function yields the total ideal thermodynamic function.

3. THE PUBCO-I CODE

3.1 General Features

The IBM cards used at the Los Alamos Scientific Laboratory are punched in columns 1 to 36 and 38 to 72. All discussion will be based upon this punching convention.

The code uses decimal floating point and fixed point numbers for numerical input and Hollerith alphameric characters as binary coded decimal (BCD) data for molecular identification. The output is printed by the SHARE-2 board as floating point numbers for all molecular input data and as fixed point numbers for all computational data, i.e., temperature and thermodynamic functions. The molecular formula is printed as Hollerith characters.

Seven Los Alamos subroutines and one Los Alamos auxiliary program are used in the course of the program. They will be identified below and

discussed in detail in the following section. The identification and function of each subroutine is as follows:

LAS-001	Fixed decimal input
LAS-011	Floating decimal input
LAS-020	Binary card loader
LAS-117	General on-off line print
LAS-800	Square root
LAS-816	Floating exponential
LAS-820	Floating natural logarithm
LAA-027	Binary correction card loader

The computation of the thermodynamic functions is performed in two parts. The rigid rotator-harmonic oscillator functions are calculated for all molecules. If the more exact nonrigid rotator-anharmonic oscillator functions are desired, sense switch No. 1 is depressed on the console at the beginning of the computation. The activation of this sense switch causes the IBM 704 to transfer to the portion of the code that computes the nonrigid rotator-anharmonic oscillator correction terms to the thermodynamic functions, rather than to the print routine as would normally be done.

3.2 Subroutines

Since the writeups for some of the subroutines used in the PUBCO-I code are rather lengthy, only those portions of the writeups which are necessary for the proper utilization of these subroutines will be covered in this report. The various error stops associated with these subroutines are listed in Section 3.3.

LAS-001. This program loads blocks of ten digit, fixed decimal constants. It is identified in the code as region 708 and is necessary only when the nonrigid rotator-anharmonic oscillator treatment is used. Its only function

is to load the number of vibration-rotation interactions to be considered for a specific molecule. It is entered by means of a transition card. This transition card and the one used with LAS-011 are punched in columns 1 and 2 in the "9" row. The binary location to which the transition is to be made is punched in the "9" row in the appropriate columns from column 22 to column 36. LAS-001 requires a transition to $(4070)_8$ in order to be entered. Two decimally punched cards are required when this subroutine is used, a control card and a data card.

The control card must be punched as follows:

<u>Card Column</u>	<u>Punch</u>	<u>Significance</u>
1	8	Control card
2-6	$(03220)_{10}$	Initial loading address
7-11	Blank	Increment
12-13	$(02)_{10}$	Decimal exponent
14-15	$(17)_{10}$	Binary scale factor

The data card must be punched as follows:

<u>Column</u>	<u>Punch</u>
1	Blank
2	0 (unless there are 10 or more vibration-rotation interaction terms)
3	Number of vibration-rotation interaction terms
4-11	0

LAS-011. Blocks of eight digit, floating decimal constants (up to seven per card) are loaded by means of this subroutine. It is identified in the code as region 707 and is used to load all molecular data for the problem. It is entered by means of a transition card transferring control to $(3472)_8$

for the first problem of a series and by means of a basic linkage-calling routine in region 107.29(2304)₈ for all problems except the first of a series. Each group of molecular data requires a control card and one or more data cards.

The control card must be punched as follows:

<u>Card Columns</u>	<u>Punch</u>	<u>Significance</u>
1	8	Control card
2-6	FWA	Initial loading address

The data cards must be punched as follows:

<u>Card Columns</u>	<u>Punch</u>	<u>Significance</u>
1	Blank	Data card
2-9	N ₁	1st number
10-11	E ₁	1st exponent
12-19	N ₂	2nd number
20-21	E ₂	2nd exponent
22-29	N ₃	3rd number
30-31	E ₃	3rd exponent
32-36	N ₄	First five digits of 4th number
37	Blank	
38-40	N ₄	Last three digits of 4th number
41-42	E ₄	4th exponent
43-50	N ₅	5th number
51-52	E ₅	5th exponent
53-60	N ₆	6th number
61-62	E ₆	6th exponent
63-70	N ₇	7th number
71-72	E ₇	7th exponent

All zeros must be punched. If fewer than seven numbers are on a data card, the unused field must be left blank. Numbers must be punched consecutively, starting at the left of the card. The signs of the numbers and exponents are punched over the first digit of the number and of the exponent, respectively. An 11 punch is used for minus but no additional punch is used to designate a positive number.

The following initial loading addresses are required in the program:

(00651) ₁₀	Rigid rotator-harmonic oscillator data
(03140) ₁₀	Stretching and vibration-rotation interaction constants
(03155) ₁₀	Anharmonicity constants

LAS-020. This program loads ordinary binary cards by means of a calling sequence at $107.28(2301)_8$ and returns control to the main program at $(2302)_8$ when it reads a blank card. Therefore, even if no binary cards are to be loaded in a particular problem (as will normally be the case), it is necessary to put a blank card in the deck at the appropriate spot in order to return control to the main program at $(2302)_8$.

LAS-117. This program prints fixed and/or floating decimal numbers either on-line or off-line. It is used to print on-line in PUBCO-I, but it can be modified by 027 correction cards to print off-line. These changes will be discussed later in this section. This subroutine is entered in region 100 at $100.0(1375)_8$ and $100.1(1401)_8$ to print molecular data in floating point for rigid rotator-harmonic oscillator molecules and also at $100.14(1416)_8$, $100.22(1426)_8$, $100.26(1432)_8$, and $100.36(1444)_8$ for nonrigid rotator-anharmonic oscillator molecules.

For RRHO molecules, the molecular data which are stored in 802.1 to 802.67 are printed consecutively (seven words per line). For NRRAO molecules, the 802 block is printed as before, followed by the vibration-rotation interaction constants in 804.1 to 804.11 (five words per line), the stretching

constant in 804.0 (one word per line), and the anharmonicity constants in 805.0 to 805.55 (seven words per line). The temperature, the free energy function, enthalpy function, entropy, and heat capacity are printed in this order on one line as fixed point numbers after the computation of the thermodynamic functions has been performed at each desired temperature. The thermodynamic functions are printed with five significant figures following the decimal point; since most spectroscopic data are not sufficiently accurate to permit this degree of precision, it will be desirable in most cases for the user to round off the thermodynamic functions to the appropriate number of figures for a given molecule. The molecular formula is printed at the head of the molecular data and at the head of the thermodynamic functions.

The following changes in the program are required to print off-line with the same format as the on-line printing. The octal designation for the operation PTW is +200000.

<u>Location</u>	<u>Operation</u>	<u>Address</u>	<u>Tag</u>	<u>Decrement</u>
(1376) ₈	PTW	0	0	(2) ₈
(1411) ₈	PTW	0	0	(60) ₈
(1424) ₈	PTW	0	0	(60) ₈
(1430) ₈	PTW	0	0	0
(1442) ₈	PTW	0	0	(60) ₈
(1446) ₈	PTW	0	0	(1) ₈
(2221) ₈	PTW	0	0	(60) ₈

LAS-800. This program, which is entered at α by a basic linkage, takes the square root of a normalized number, x , in the accumulator and returns to the main program at $\alpha + 2$ with $\sqrt{x}$ in the accumulator. If the $x \leq 0$, the return is to $\alpha + 1$ with $\sqrt{|x|}$ in the accumulator. The PUBCO code is set up to give a program stop at all $\alpha + 1$ positions in the square

root subroutine since there is no situation where x should be a negative number. The square root subroutine is identified in the code as region 701.

LAS-816. This subroutine evaluates the exponential of a floating point number, x , in the accumulator. The 704 requires that $|x| < 87.3$. The entry is at α with x in the accumulator and the normal exit is at $\alpha + 2$ with e^x in the accumulator. Since exponent overflows are possible in the program, the exit for this condition at $\alpha + 1$ is set up to store 10^{30} in the accumulator if $x > 87.3$ and 0 if $x < -87.3$. This subroutine is region 704 of the code.

LAS-820. This program evaluates the natural logarithm of a normalized floating point number, $x > 0$. Entry to the program is at α with x in the accumulator and the normal exit is at $\alpha + 2$ with $\ln x$ in the accumulator. If $x \leq 0$, the exit is at $\alpha + 1$. Some of the $\alpha + 1$ exits are programmed as "halts" while others are "halt and proceed"; the instruction used in a particular calling sequence depends upon whether x can physically be zero in that particular situation. LAS-820 is identified as region 702 in the code.

LAA-027. This self-loading auxiliary routine for binary correction cards is used to load the molecular formula into the IBM 704. The card bearing the molecular identification for a given problem is loaded into $802.0(1212)_8$ by LAA-027 after the corresponding decimal data for that problem have been loaded. The BCD punched alphameric characters are punched in columns 38 to 72. Binary punched correction cards also can be loaded by LAA-027 if it becomes necessary to change some of the instructions of the code itself.

3.3 Error Stops

All the error stops in the PUBCO-I noncomputing subroutines are listed sequentially below along with comments giving the reason for their occurrence.

The error stops in the three computing subroutines have already been discussed.

<u>Location</u>		<u>Significance</u>
(1831) ₁₀	(3447) ₈	Check sum disagreement in LAS-020. (Press START button to read next card)
(2101) ₁₀	(4065) ₈	Data card punched incorrectly in LAS-011
(2332) ₁₀	(4434) ₈	Data card punched incorrectly in LAS-001

3.4 Regions within the Code

The code is composed of thirty-six regions, ten of which are used as operational regions, twelve of which are used for temporary storage of computational results, seven of which are occupied by the previously discussed subroutines, and seven of which contain input data. These four groups of regions are identified, respectively, by 100, 600, 700, and 800 series region numbers with the exception of subroutine erasable storage, which is identified as region 1.

The following list gives the function of each of these regions, except those of the 700 series which have been discussed already.

<u>Region</u>	<u>Function</u>
1	Subroutine erasable storage
100	Print input data
102	Calculate translation and electronic contributions to thermodynamic functions
103	Calculate vibrational contributions
104	Calculate nonlinear rotational contributions
105	Calculate linear rotational contributions
106	Print output of computations
107	Increment temperature

<u>Region</u>	<u>Function</u>
108	Calculate stretching contributions
109	Calculate vibration-rotation contributions
110	Calculate anharmonicity contributions
600	Temporary storage for translation and rotation calculations
601	Temporary storage for vibration calculations
602	Temporary storage for stretching calculations
603	Temporary storage for vibration-rotation calculations
604	Temporary storage for ν_{ij} terms
605	Temporary storage for anharmonicity calculations
606	Temporary storage for B'_{ij}
607	Temporary storage for A_{ij}
608	Temporary storage for A'_{ij}
609	Temporary storage for A''_{ij}
610	Temporary storage for B_{ij}
800	Input storage for physical constants
801	Input storage for numerical constants
802	Input storage for rigid rotator-harmonic oscillator data
803	Input storage for temperatures
804	Input storage for stretching and vibration-rotation constants
805	Input storage for anharmonicity constants
806	Input storage for manipulating ij routines

3.5 Input Data

Because the possibility exists that an individual may want to change one or more pieces of input data, some discussion of the data now stored in the code will be given.

The 800 block contains the values of the physical constants needed in

the computation. The constants are those of Cohen, et al.,⁶ with the exception of data pertaining to the gas constant, R, and the Boltzmann constant, k, which are based upon constants used by the National Bureau of Standards.

The order of the physical constants in region 800 is as follows:

<u>Region</u>	<u>Function</u>
800.0	Gas constant, R
800.1	π
800.2	Boltzmann constant, k
800.3	Planck constant, h
800.4	Velocity of light, c
800.5	Avogadro number, N
800.6	Pressure in dynes/cm ²
800.7	Sackur-Tetrode constant
800.8	$5/2 R$
800.9	$R \ln P$
800.10	$3/2 R$
800.11	hc/k

The 801 block contains numbers needed in the calculations and will not be discussed.

The 802 block contains molecular data in the following order:

<u>Region</u>	<u>Function</u>
802.0	Molecular formula
802.1	Molecular weight
802.2	Symmetry number
802.3	Electronic multiplicity
802.4	Rotational constant A

<u>Region</u>	<u>Function</u>
802.5	Rotational constant B
802.6	Rotational constant C
802.7	Wave number of 1st fundamental vibrational frequency, ν_1
802.8	Vibrational degeneracy of ν_1 (g_1)
802.9	Wave number of 2nd fundamental vibrational frequency, ν_2
802.10	Vibrational degeneracy of ν_2 (g_2)

The loading of the molecular formula into 802.0 by LAA-027 has been discussed previously.

The code presently is arranged to handle twenty-five different vibrational frequencies but it has sufficient storage in region 802 to accommodate five additional frequencies and their associated degeneracies. If this change is made, certain corresponding indexing changes also must be made in region 103. One should load the ν_i 's and g_i 's required for a given molecule consecutively starting at 802.7; it is not necessary to load zeros beyond the last g_i which is used in the problem.

Region 803 has various temperatures and temperature increments stored in it so that the code will compute the thermodynamic functions at 50°K intervals from 50°K to 250°K, at 298.16°K, and at 100°K intervals from 300°K through 5000°K. The initial temperature is stored at 803.0; the initial ΔT is at 803.1; the second ΔT is stored at 803.4; and the final test temperature is stored at 803.6. New temperatures can be stored in this region by means of LAS-011 if one wishes to change the temperature scanning routine.

The stretching constant, ρ , is stored in 804.0 and the vibration-rotation interaction constants, δ_i , are stored in 804.1 to 804.14. If more than fourteen δ_i 's are required for a problem, it will be necessary to reassemble the code.

The anharmonicity constants, X_{ij} , are stored in region 805. Space has

been allotted for sixty-five of these constants within this region. The X_{ij} 's must be loaded consecutively from 805.0 in the order $X_{11}, X_{12}, X_{13}, \dots, X_{1j}, X_{22}, X_{23}, \dots, X_{2j}, X_{33}, \dots, X_{3j}, \dots, X_{jj}$. It is required that $i \leq j$.

Region 806 contains certain indexing constants necessary to carry out the calculations correctly, as well as 10^{30} , which is used when the exponential operation causes the 704 to overflow. If not more than twenty-five vibrational frequencies are used in a problem, it will be necessary to change only 806.0 when one is treating nonrigid rotator-anharmonic oscillator molecules. The number in 806.0 is loaded by LAS-001 and must be equal to the number of different vibrational frequencies for the particular molecule which is being computed; i.e., three for HCN and five for C_2H_2 .

3.6 The PUBCO-I Deck

The PUBCO-I deck is formed by the following cards:

LAA-020 self-loading binary card

PUBCO-I binary cards

TNX to $(3472)_8$ transition card (to LAS-011.10)

LAS-011 control card for 802 block of data

Decimal data cards for 802 block

LAS-011 control card for 804 block of data

Decimal data card(s) for 804 block

LAS-011 control card for 805 block of data

Decimal data card(s) for 805 block

TNX to $(4070)_8$ transition card (to LAS-001.14)

LAS-001 control card for 806.0

Decimal data card for 806.0

} Only for NRRAO molecules

LAA-027 self-loading correction card

Binary card with molecular formula in $(1212)_8$

TNX to $(1375)_8$ transition card (to start of problem)

Binary cards (if any)

Blank card

When several molecules are being computed as a group, the deck should have the following cards for each molecule after the first:

LAS-011 control card for 802 block of data

Decimal data cards for 802 block

LAS-011 control card for 804 block of data

Decimal data card(s) for 804 block

LAS-011 control card for 805 block of data

Decimal data card(s) for 805 block

TNX to $(4070)_8$ transition card

LAS-001 control card for 806.0

Decimal data card for 806.0

} If NRRAO molecule

LAA-027 self-loading correction card

Binary card with molecular formula in $(1212)_8$

TNX to $(1375)_8$ transition card

Binary cards (if any)

Blank card

2 blank cards after the blank card for the last molecule in the group.

REFERENCES

1. G. Herzberg, Molecular Spectra and Molecular Structure, II. Infrared and Raman Spectra of Polyatomic Molecules., pp. 501-526, D. Van Nostrand Company, Inc., New York, 1945.
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3. A. S. Friedman and L. Haar, "High Speed Machine Computation of Ideal Gas Thermodynamic Functions. I. The Isotopic Water Molecules", J. Chem. Phys., 22, 2051-2058 (1954).
4. J. C. Bradley, L. Haar, and A. S. Friedman, "Ideal Gas Thermodynamic Functions of the Isotopic Hydrogen Cyanides", National Bureau of Standards Report NBS-4161, 1955.
5. R. E. Pennington and K. A. Kobe, "Contributions of Vibrational Anharmonicity and Rotation-Vibration Interaction to Thermodynamic Functions", J. Chem. Phys., 22, 1442-1447 (1954).
6. E. R. Cohen, J. W. M. DuMond, T. W. Layton, and J. S. Rollett, "Analysis of Variance of the 1952 Data on the Atomic Constants and a New Adjustment, 1955", Revs. Modern Phys., 27, 363-380 (1955).

Appendix A
IBM 704 LISTING FOR PUBCO-I CODE

ORIGIN TABLE.	SYMBOL.FWA	SYMBOL.LWA	OCT.FWA	LWA	DECIM.FWA	LWA
	1.0000.	1.3107.1	700	77777	448	32767
	800.0000.	800.3107.1	1130	77777	600	32767
	801.0000.	801.3107.1	1154	77777	620	32767
	802.0000.	802.3107.1	1212	77777	650	32767
	601.0000.	601.3107.1	1332	77777	730	32767
	803.0000.	803.3107.1	1356	77777	750	32767
	100.0000.	100.0041.	1375	1460	765	816
	102.0000.	102.0021.	1464	1512	820	842
	103.0000.	103.0067.	1522	1632	850	922
	104.0000.	104.0116.	1642	2031	930	1049
	105.0000.	105.0077.	2044	2161	1060	1137
	106.0000.	106.0029.	2203	2237	1155	1183
	107.0000.	107.0030.	2241	2305	1185	1221
	600.0000.	600.3107.1	2311	77777	1225	32767
	701.0000.	701.3107.1	2342	77777	1250	32767
	702.0000.	702.3107.1	2373	77777	1275	32767
	703.0000.	703.3107.1	2450	77777	1320	32767
	704.0000.	704.3107.1	3314	77777	1740	32767
	706.0000.	706.3107.1	3422	77777	1810	32767
	707.0000.	707.3107.1	3460	77777	1840	32767
	708.0000.	708.3107.1	4052	77777	2090	32767
	108.0000.	108.0035.	4420	4466	2320	2358
	109.0000.	109.0118.	4475	4670	2365	2488
	110.0000.	110.0209.	4711	5211	2505	2697
	602.0000.	602.3107.1	5233	77777	2715	32767
	603.0000.	603.3107.1	5245	77777	2725	32767
	604.0000.	604.3107.1	5271	77777	2745	32767
	605.0000.	605.3107.1	5372	77777	2810	32767
	606.0000.	606.3107.1	5423	77777	2835	32767
	607.0000.	607.3107.1	5524	77777	2900	32767
	608.0000.	608.3107.1	5620	77777	2960	32767
	609.0000.	609.3107.1	5714	77777	3020	32767
	610.0000.	610.3107.1	6010	77777	3080	32767
	804.0000.	804.3107.1	6104	77777	3140	32767
	805.0000.	805.3107.1	6123	77777	3155	32767
	806.0000.	806.3107.1	6224	77777	3220	32767

02342 LAS	002371	000700	7	701. 0000.	LAS 800. 2893.	1. 0003.	NORMAL EXIT=(A+2) LG	1250	2342
02373 LAS	002441	000700	7	702. 0000.	LAS 820. 0000.	1. 0002.	FL PT LOG BASE E	1275	2373
02450 LAS	003267	000700	7	703. 0000.	LAS 117. 0000.	1. 0051.	GEN ON-OFF LINE PRINT	1320	2450
03314 LAS	003412	000700	7	704. 0000.	LAS 816. 5770.	1. 0005.	FASTER EXP 2.5 MS	1740	3314
03422 LAS	003447	000700	7	706. 0000.	LAS 20. 3400.	1. 0000.	STOP R 21 CH SUM ERRO	1810	3422
03460 LAS	004035	000700	7	707. 0000.	LAS 11. 0000.	1. 0023.	FLOATING DEC INPUT	1840	3460
04052 LAS	004402	000700	7	708. 0000.	LAS 1. 0000.	1. 0025.	FIXED DEC INPUT	2090	4052

01375	TSX	007400	402450	100.	0000.	TSX	703.	0000.	C	0.	0000.	765	1375
01376	PTH	302046	001212	100.	0000.1	PTH	802.	0000.		0.	1062.	766	1376
01377	PON	100000	000362	100.	0000.2	PON	0.	0242.		0.	0000.	767	1377
01400	SDX	-053400	101456	100.	0000.3	SDX	2.	0039.	A	0.	0000.	768	1400
01401	TSX	007400	402450	100.	0001.	TSX	703.	0000.	C	0.	0000.	769	1401
01402	SVN	-317521	101315	100.	0002.	SVN	802.	0067.	A	0.	8017.	770	1402
01403	SVN	-317542	101316	100.	0003.	SVN	802.	0068.	A	0.	8034.	771	1403
01404	SVN	-317563	101317	100.	0004.	SVN	802.	0069.	A	0.	8051.	772	1404
01405	SVN	-317604	101320	100.	0005.	SVN	802.	0070.	A	0.	8068.	773	1405
01406	SVN	-317625	101321	100.	0006.	SVN	802.	0071.	A	0.	8085.	774	1406
01407	SVN	-317646	101322	100.	0007.	SVN	802.	0072.	A	0.	8102.	775	1407
01410	SVN	-317667	101323	100.	0008.	SVN	802.	0073.	A	0.	8119.	776	1410
01411	PON	100000	000000	100.	0009.	PON	0.	0000.		0.	0000.	777	1411
01412	TX	200007	101401	100.	0010.	TX	2.	0001.	A	0.	0007.	778	1412
01413	SE	076000	000161	100.	0011.	SE	0.	0113.		0.	0000.	779	1413
01414	T	002000	001444	100.	0012.	T	2.	0036.		0.	0000.	780	1414
01415	SDX	-053400	101457	100.	0013.	SDX	2.	0040.	A	0.	0000.	781	1415
01416	TSX	007400	402450	100.	0014.	TSX	703.	0000.	C	0.	0000.	782	1416
01417	SVN	-317524	106113	100.	0015.	SVN	804.	0007.	A	0.	8020.	783	1417
01420	SVN	-317550	106114	100.	0016.	SVN	804.	0008.	A	0.	8040.	784	1420
01421	SVN	-317574	106115	100.	0017.	SVN	804.	0009.	A	0.	8060.	785	1421
01422	SVN	-317620	106116	100.	0018.	SVN	804.	0010.	A	0.	8080.	786	1422
01423	SVN	-317644	106117	100.	0019.	SVN	804.	0011.	A	0.	8100.	787	1423
01424	PON	100000	000000	100.	0020.	PON	0.	0000.		0.	0000.	788	1424
01425	TX	200005	101416	100.	0021.	TX	2.	0014.	A	0.	0005.	789	1425
01426	TSX	007400	402450	100.	0022.	TSX	703.	0000.	C	0.	0000.	790	1426
01427	SVN	-317562	006104	100.	0023.	SVN	804.	0000.		0.	8050.	791	1427
01430	PON	100364	000000	100.	0024.	PON	0.	0000.		0.	0244.	792	1430
01431	SDX	-053400	101460	100.	0025.	SDX	2.	0041.	A	0.	0000.	793	1431
01432	TSX	007400	402450	100.	0026.	TSX	703.	0000.	C	0.	0000.	794	1432
01433	SVN	-317521	106205	100.	0027.	SVN	805.	0050.	A	0.	8017.	795	1433
01434	SVN	-317542	106206	100.	0028.	SVN	805.	0051.	A	0.	8034.	796	1434
01435	SVN	-317563	106207	100.	0029.	SVN	805.	0052.	A	0.	8051.	797	1435
01436	SVN	-317604	106210	100.	0030.	SVN	805.	0053.	A	0.	8068.	798	1436
01437	SVN	-317625	106211	100.	0031.	SVN	805.	0054.	A	0.	8085.	799	1437
01440	SVN	-317646	106212	100.	0032.	SVN	805.	0055.	A	0.	8102.	800	1440
01441	SVN	-317667	106213	100.	0033.	SVN	805.	0056.	A	0.	8119.	801	1441
01442	PON	100000	000000	100.	0034.	PON	0.	0000.		0.	0000.	802	1442
01443	TX	200007	101432	100.	0035.	TX	2.	0026.	A	0.	0007.	803	1443
01444	TSX	007400	402450	100.	0036.	TSX	703.	0000.	C	0.	0000.	804	1444
01445	PTH	302046	001212	100.	0036.1	PTH	802.	0000.		0.	1062.	805	1445
01446	PON	100000	000361	100.	0037.	PON	0.	0241.		0.	0000.	806	1446
01447	CA	050000	001215	100.	0037.1	CA	802.	0003.		0.	0000.	807	1447
01450	TSX	007400	402373	100.	0037.2	TSX	702.	0000.	C	0.	0000.	808	1450
01451	ZS	060000	001215	100.	0037.3	ZS	802.	0003.		0.	0000.	809	1451
01452	LR	076500	000043	100.	0037.4	LR	0.	0035.		0.	0000.	810	1452
01453	FM	026000	001130	100.	0037.5	FM	800.	0000.		0.	0000.	811	1453
01454	ST	060100	001215	100.	0037.6	ST	802.	0003.		0.	0000.	812	1454
01455	T	002000	001464	100.	0038.	T	102.	0000.		0.	0000.	813	1455
01456		000102	000000	100.	0039.		0.	0000.		0.	0066.	814	1456
01457		000006	000000	100.	0040.		0.	0000.		0.	0006.	815	1457
01460		000062	000000	100.	0041.		0.	0000.		0.	0050.	816	1460

MOLECULE IDENTIFICAT.
HALF PAGE

LAS 117 PRINT FLTG
RIGID
ROTATOR-
HARMONIC
OSCILLATOR
DATA

SS NO. 1
CALC TRANS.

DELTAS

STRETCH CONSTANT

ANHARMONICITY
CONSTANTS

MOLECULE IDENTIFICAT.

MULTIPLICITY
LN

R
R LN MULT.
CALC TRANS.

01464	CA	050000	001356	102.	0000.	CA	803.	0000.	0.	0000.	T ZERO	820	1464	
01465	ST	060100	000735	102.	0001.	ST	1.	0029.	0.	0000.	T WKG	821	1465	
01466	TSX	007400	402373	102.	0002.	TSX	702.	0000.	C	0.	0000.	LN	822	1466
01467	H	000000	000000	102.	0003.	H	0.	0000.	0.	0000.		823	1467	
01470	LR	076500	000043	102.	0004.	LR	0.	0035.	0.	0000.		824	1470	
01471	FM	026000	001140	102.	0005.	FM	800.	0008.	0.	0000.	5/2 R	825	1471	
01472	ST	060100	002311	102.	0006.	ST	600.	0000.	0.	0000.	LN T	826	1472	
01473	CA	050000	001213	102.	0007.	CA	802.	0001.	0.	0000.	MW	827	1473	
01474	TSX	007400	402373	102.	0008.	TSX	702.	0000.	C	0.	0000.	LN	828	1474
01475	H	000000	000000	102.	0009.	H	0.	0000.	0.	0000.		829	1475	
01476	LR	076500	000043	102.	0010.	LR	0.	0035.	0.	0000.		830	1476	
01477	FM	026000	001142	102.	0011.	FM	800.	0010.	0.	0000.	3/2 R LN M	831	1477	
01500	FA	030000	002311	102.	0012.	FA	600.	0000.	0.	0000.		832	1500	
01501	FA	030000	001137	102.	0013.	FA	800.	0007.	0.	0000.	S-T CONST	833	1501	
01502	FS	030200	001141	102.	0014.	FS	800.	0009.	0.	0000.	R LN P	834	1502	
01503	FA	030000	001215	102.	0014.1	FA	802.	0003.	0.	0000.	R LN MULT.	835	1503	
01504	ST	060100	000736	102.	0015.	ST	1.	0030.	0.	0000.	-F/T TRANS	836	1504	
01505	FA	030000	001140	102.	0016.	FA	800.	0008.	0.	0000.	5/2 R	837	1505	
01506	ST	060100	000740	102.	0017.	ST	1.	0032.	0.	0000.	S TRANS	838	1506	
01507	CA	050000	001140	102.	0018.	CA	800.	0008.	0.	0000.		839	1507	
01510	ST	060100	000737	102.	0019.	ST	1.	0031.	0.	0000.	H/T TRANS	840	1510	
01511	ST	060100	000741	102.	0020.	ST	1.	0033.	0.	0000.	C SUB P	841	1511	
01512	T	002000	001522	102.	0021.	T	103.	0000.	0.	0000.	CALC v1B FN	842	1512	

01522	SDX	-053400	201630	103.	0000.	SDX	2.	0065.	B	0.	0000.		850	1522
01523	CA	050000	201304	103.	0001.	CA	802.	0058.	B	0.	0000.	G SUB EYE	851	1523
01524	TZ	010000	001607	103.	0002.	TZ	2.	0052.	0.	0000.	PAST LAST NU	852	1524	
01525	LQ	056000	001143	103.	0003.	LQ	800.	0011.	0.	0000.	HC/K	853	1525	
01526	FM	026000	201303	103.	0004.	FM	802.	0057.	B	0.	0000.	NU SUB EYE	854	1526
01527	FD	024000	000735	103.	0005.	FD	1.	0029.	0.	0000.	T	855	1527	
01530	SQ	-060000	001332	103.	0006.	SQ	601.	0000.	0.	0000.	HC NU/KT	856	1530	
01531	CS	050200	001332	103.	0007.	CS	601.	0000.	0.	0000.		857	1531	
01532	TSX	007400	403314	103.	0008.	TSX	704.	0000.	C	0.	0000.	E TO - HCNU/KT	858	1532
01533	T	002000	001631	103.	0009.	T	2.	0066.	0.	0000.	EXP GR THAN 88	859	1533	
01534	ST	060100	001332	103.	0010.	ST	601.	0000.	0.	0000.		860	1534	
01535	CA	050000	001155	103.	0011.	CA	801.	0001.	0.	0000.	ONE	861	1535	
01536	FS	030200	001332	103.	0012.	FS	601.	0000.	0.	0000.		862	1536	
01537	ST	060100	001333	103.	0013.	ST	601.	0001.	0.	0000.	1-E TO -X	863	1537	
01540	TSX	007400	402373	103.	0014.	TSX	702.	0000.	C	0.	0000.	LN	864	1540
01541	H	000000	000000	103.	0015.	H	0.	0000.	0.	0000.		865	1541	
01542	ST	060100	001334	103.	0016.	ST	601.	0002.	0.	0000.	OF ABOVE	866	1542	
01543	LQ	056000	001334	103.	0017.	LQ	601.	0002.	0.	0000.		867	1543	
01544	FM	026000	201304	103.	0018.	FM	802.	0058.	B	0.	0000.	G	868	1544
01545	LR	076500	000043	103.	0019.	LR	0.	0035.	0.	0000.		869	1545	
01546	FM	026000	001130	103.	0020.	FM	800.	0000.	0.	0000.	R	870	1546	
01547	CHS	076000	000002	103.	0021.	CHS	0.	0000.	0.	0000.		871	1547	

01550 ST	060100	001335	103.	0022.	ST	601.	0003.	0.	0000.	-F/T VIB	872	1550	
01551 LQ	056000	001332	103.	0023.	LQ	601.	0000.	0.	0000.		873	1551	
01552 FM	026000	201303	103.	0024.	FM	802.	0057.	B	0.	0000.	NU	874	1552
01553 FD	024000	001333	103.	0025.	FD	601.	0001.		0.	0000.		875	1553
01554 FM	026000	201304	103.	0026.	FM	802.	0058.	B	0.	0000.	G	876	1554
01555 LR	076500	000043	103.	0027.	LR	0.	0035.		0.	0000.		877	1555
01556 FM	026000	001143	103.	0028.	FM	800.	0011.		0.	0000.	HC/K	878	1556
01557 FD	024000	000735	103.	0029.	FD	1.	0029.		0.	0000.	T	879	1557
01560 FM	026000	001130	103.	0030.	FM	800.	0000.		0.	0000.	R	880	1560
01561 ST	060100	001336	103.	0031.	ST	601.	0004.		0.	0000.	H/T VIB	881	1561
01562 FA	030000	001335	103.	0032.	FA	601.	0003.		0.	0000.		882	1562
01563 ST	060100	001337	103.	0033.	ST	601.	0005.		0.	0000.	S VIB	883	1563
01564 LQ	056000	001336	103.	0034.	LQ	601.	0004.		0.	0000.		884	1564
01565 FM	026000	201303	103.	0035.	FM	802.	0057.	B	0.	0000.	NU	885	1565
01566 FD	024000	001333	103.	0036.	FD	601.	0001.		0.	0000.		886	1566
01567 FM	026000	001143	103.	0037.	FM	800.	0011.		0.	0000.	HC/K	887	1567
01570 FD	024000	000735	103.	0037.1	FD	1.	0029.		0.	0000.		888	1570
01571 SQ	060000	001340	103.	0038.	SQ	601.	0006.		0.	0000.	C SUB P VIB	889	1571
01572 CA	050000	001335	103.	0039.	CA	601.	0003.		0.	0000.	-F SUB SUMS	890	1572
01573 FA	030000	001341	103.	0040.	FA	601.	0007.		0.	0000.		891	1573
01574 ST	060100	001341	103.	0041.	ST	601.	0007.		0.	0000.	-F/T VIB TOT	892	1574
01575 CA	050000	001336	103.	0042.	CA	601.	0004.		0.	0000.		893	1575
01576 FA	030000	001342	103.	0043.	FA	601.	0008.		0.	0000.		894	1576
01577 ST	060100	001342	103.	0044.	ST	601.	0008.		0.	0000.	H/T VIB TOT	895	1577
01600 CA	050000	001337	103.	0045.	CA	601.	0005.		0.	0000.		896	1600
01601 FA	030000	001343	103.	0046.	FA	601.	0009.		0.	0000.		897	1601
01602 ST	060100	001343	103.	0047.	ST	601.	0009.		0.	0000.	S VIB TOT	898	1602
01603 CA	050000	001340	103.	0048.	CA	601.	0006.		0.	0000.		899	1603
01604 FA	030000	001344	103.	0049.	FA	601.	0010.		0.	0000.		900	1604
01605 ST	060100	001344	103.	0050.	ST	601.	0010.		0.	0000.	C SUB P TOT	901	1605
01606 TX	200002	201523	103.	0051.	TX	2.	0001.	B	0.	0002.	FREQ TEST	902	1606
01607 CA	050000	001341	103.	0052.	CA	601.	0007.		0.	0000.		903	1607
01610 FA	030000	000736	103.	0053.	FA	1.	0030.		0.	0000.	-F/T TRANS	904	1610
01611 ST	060100	000736	103.	0054.	ST	1.	0030.		0.	0000.	PLUS VIB	905	1611
01612 CA	050000	001342	103.	0055.	CA	601.	0008.		0.	0000.		906	1612
01613 FA	030000	000737	103.	0056.	FA	1.	0031.		0.	0000.	H/T TRANS	907	1613
01614 ST	060100	000737	103.	0057.	ST	1.	0031.		0.	0000.	PLUS VIB	908	1614
01615 CA	050000	001343	103.	0058.	CA	601.	0009.		0.	0000.		909	1615
01616 FA	030000	000740	103.	0059.	FA	1.	0032.		0.	0000.	S TRANS	910	1616
01617 ST	060100	000740	103.	0060.	ST	1.	0032.		0.	0000.	PLUS VIB	911	1617
01620 CA	050000	001344	103.	0061.	CA	601.	0010.		0.	0000.		912	1620
01621 FA	030000	000741	103.	0062.	FA	1.	0033.		0.	0000.	C SUB P TR	913	1621
01622 ST	060100	000741	103.	0063.	ST	1.	0033.		0.	0000.	PLUS VIB	914	1622
01623 ZS	060000	001341	103.	0064.	ZS	601.	0007.		0.	0000.	STORE ZERO	915	1623
01624 ZS	060000	001342	103.	0064.1	ZS	601.	0008.		0.	0000.		916	1624
01625 ZS	060000	001343	103.	0064.2	ZS	601.	0009.		0.	0000.		917	1625
01626 ZS	060000	001344	103.	0064.3	ZS	601.	0010.		0.	0000.		918	1626
01627 T	002000	001642	103.	0064.4	T	104.	0000.		0.	0000.	CALC ROT FNS	919	1627
01630	000062	000000	103.	0065.		0.	0000.		0.	0050.		920	1630
01631 CA	050000	001154	103.	0066.	CA	801.	0000.		0.	0000.	ZERO	921	1631
01632 T	002000	001534	103.	0067.	T	2.	0010.		0.	0000.		922	1632

01642	CA	050000	001216	104.	0000.	CA	802.	0004.	0.	0000.	A	930	1642
01643	TZ	010000	002044	104.	0001.	TZ	105.	0000.	0.	0000.	LINEAR	931	1643
01644	CA	050000	001143	104.	0005.	CA	800.	0011.	0.	0000.	HC/K	932	1644
01645	FD	024000	000735	104.	0006.	FD	1.	0029.	0.	0000.		933	1645
01646	SQ	-060000	002311	104.	0007.	SQ	600.	0000.	0.	0000.	HC/KT	934	1646
01647	LQ	056000	001217	104.	0008.	LQ	802.	0005.	0.	0000.	B	935	1647
01650	FM	026000	001220	104.	0009.	FM	802.	0006.	0.	0000.	C	936	1650
01651	TSX	007400	402342	104.	0010.	TSX	701.	0000.	C	0.	SQ RT	937	1651
01652	H	000000	000000	104.	0011.	H	0.	0000.	0.	0000.		938	1652
01653	ST	060100	002312	104.	0012.	ST	600.	0001.	0.	0000.	OF BC	939	1653
01654	LQ	056000	002311	104.	0013.	LQ	600.	0000.	0.	0000.		940	1654
01655	FM	026000	001165	104.	0014.	FM	801.	0009.	0.	0000.	1/4	941	1655
01656	LR	076500	000043	104.	0015.	LR	0.	0035.	0.	0000.		942	1656
01657	FM	026000	002312	104.	0016.	FM	600.	0001.	0.	0000.		943	1657
01660	TSX	007400	403314	104.	0017.	TSX	704.	0000.	C	0.	E TO	944	1660
01661	H	000000	000000	104.	0018.	H	0.	0000.	0.	0000.		945	1661
01662	ST	060100	002313	104.	0019.	ST	600.	0002.	0.	0000.	BCHC/4KT	946	1662
01663	LQ	056000	002311	104.	0020.	LQ	600.	0000.	0.	0000.		947	1663
01664	FM	026000	002311	104.	0021.	FM	600.	0000.	0.	0000.	SQ	948	1664
01665	ST	060100	002314	104.	0022.	ST	600.	0003.	0.	0000.		949	1665
01666	LQ	056000	002314	104.	0023.	LQ	600.	0003.	0.	0000.		950	1666
01667	FM	026000	002311	104.	0024.	FM	600.	0000.	0.	0000.	CUBED	951	1667
01670	ST	060100	002315	104.	0025.	ST	600.	0004.	0.	0000.		952	1670
01671	CA	050000	001155	104.	0026.	CA	801.	0001.	0.	0000.	ONE	953	1671
01672	FD	024000	002315	104.	0027.	FD	600.	0004.	0.	0000.		954	1672
01673	SQ	-060000	002316	104.	0028.	SQ	600.	0005.	0.	0000.	KT/HC CUBED	955	1673
01674	CA	050000	002320	104.	0029.	CA	600.	0007.	0.	0000.		956	1674
01675	TNZ	-010000	007707	104.	0030.	TNZ	2.	0040.	0.	0000.	HERE BEFORE	957	1675
01676	CA	050000	001131	104.	0031.	CA	800.	0001.	0.	0000.	P1	958	1676
01677	FD	024000	001216	104.	0032.	FD	802.	0004.	0.	0000.	A	959	1677
01700	SQ	-060000	002320	104.	0033.	SQ	600.	0007.	0.	0000.		960	1700
01701	CA	050000	002320	104.	0034.	CA	600.	0007.	0.	0000.		961	1701
01702	FD	024000	001217	104.	0035.	FD	802.	0005.	0.	0000.	B	962	1702
01703	SQ	-060000	002320	104.	0036.	SQ	600.	0007.	0.	0000.		963	1703
01704	CA	050000	002320	104.	0037.	CA	600.	0007.	0.	0000.		964	1704
01705	FD	024000	001220	104.	0038.	FD	802.	0006.	0.	0000.	C	965	1705
01706	SQ	-060000	002320	104.	0039.	SQ	600.	0007.	0.	0000.	P1/ABC	966	1706
01707	LQ	056000	002316	104.	0040.	LQ	600.	0005.	0.	0000.		967	1707
01710	FM	026000	002320	104.	0041.	FM	600.	0007.	0.	0000.		968	1710
01711	TSX	007400	402342	104.	0042.	TSX	701.	0000.	C	0.	SQ RT	969	1711
01712	H	000000	000000	104.	0043.	H	0.	0000.	0.	0000.		970	1712
01713	ST	060100	002321	104.	0044.	ST	600.	0008.	0.	0000.		971	1713
01714	CA	050000	002312	104.	0045.	CA	600.	0001.	0.	0000.	SQ RT BC	972	1714
01715	FD	024000	001216	104.	0046.	FD	802.	0004.	0.	0000.	A	973	1715
01716	SQ	-060000	002322	104.	0047.	SQ	600.	0009.	0.	0000.		974	1716
01717	CS	050200	002322	104.	0047.1	CS	600.	0009.	0.	0000.		975	1717
01720	FA	030000	001155	104.	0048.	FA	801.	0001.	0.	0000.	ONE	976	1720
01721	ST	060100	002322	104.	0049.	ST	600.	0009.	0.	0000.		977	1721
01722	LQ	056000	002321	104.	0050.	LQ	600.	0008.	0.	0000.		978	1722
01723	FM	026000	002313	104.	0051.	FM	600.	0002.	0.	0000.		979	1723
01724	ST	060100	002321	104.	0052.	ST	600.	0008.	0.	0000.		980	1724
01725	LQ	056000	002322	104.	0053.	LQ	600.	0009.	0.	0000.	1-BC/A	981	1725
01726	FM	026000	002322	104.	0054.	FM	600.	0009.	0.	0000.		982	1726
01727	ST	060100	002323	104.	0055.	ST	600.	0010.	0.	0000.	SQD	983	1727
01730	LQ	056000	002312	104.	0056.	LQ	600.	0001.	0.	0000.	SQ RT OF BC	984	1730
01731	FM	026000	002311	104.	0057.	FM	600.	0000.	0.	0000.	HC/KT	985	1731

01732	ST	060100	002324	104.	0058.	ST	600.	0011.	0.	0000.	BCHC/KT	986	1732
01733	LQ	056000	002324	104.	0059.	LQ	600.	0011.	0.	0000.		987	1733
01734	FM	026000	002324	104.	0060.	FM	600.	0011.	0.	0000.	SO	988	1734
01735	ST	060100	002325	104.	0061.	ST	600.	0012.	0.	0000.		989	1735
01736	LQ	056000	002325	104.	0062.	LQ	600.	0012.	0.	0000.		990	1736
01737	FM	026000	002323	104.	0063.	FM	600.	0010.	0.	0000.		991	1737
01740	ST	060100	002325	104.	0063.1	ST	600.	0012.	0.	0000.		992	1740
01741	FD	024000	001156	104.	0064.	FD	801.	0002.	0.	0000.	TW0	993	1741
01742	FM	026000	001164	104.	0065.	FM	801.	0008.	0.	0000.	7/240	994	1742
01743	ST	060100	002326	104.	0066.	ST	600.	0013.	0.	0000.		995	1743
01744	LQ	056000	002324	104.	0067.	LQ	600.	0011.	0.	0000.		996	1744
01745	FM	026000	002322	104.	0068.	FM	600.	0009.	0.	0000.		997	1745
01746	LR	076500	000043	104.	0069.	LR	0.	0035.	0.	0000.		998	1746
01747	FM	026000	001160	104.	0070.	FM	801.	0004.	0.	0000.	1/12	999	1747
01750	FA	030000	002326	104.	0071.	FA	600.	0013.	0.	0000.		1000	1750
01751	FA	030000	001155	104.	0072.	FA	801.	0001.	0.	0000.	ONE	1001	1751
01752	LR	076500	000043	104.	0073.	LR	0.	0035.	0.	0000.		1002	1752
01753	FM	026000	002321	104.	0074.	FM	600.	0008.	0.	0000.		1003	1753
01754	FD	024000	001214	104.	0074.1	FD	802.	0002.	0.	0000.	SIGMA	1004	1754
01755	SQ	060000	002326	104.	0075.	SQ	600.	0013.	0.	0000.		1005	1755
01756	CA	050000	002326	104.	0075.1	CA	600.	0013.	0.	0000.		1006	1756
01757	TSX	007400	402373	104.	0076.	TSX	702.	0000.	0.	0000.	C LN	1007	1757
01760	H	000000	000000	104.	0077.	H	0.	0000.	0.	0000.		1008	1760
01761	LR	076500	000043	104.	0078.	LR	0.	0035.	0.	0000.		1009	1761
01762	FM	026000	001130	104.	0079.	FM	800.	0000.	0.	0000.	R	1010	1762
01763	ST	060100	002330	104.	0080.	ST	600.	0015.	0.	0000.	-F/T ROT	1011	1763
01764	LQ	056000	002325	104.	0081.	LQ	600.	0012.	0.	0000.		1012	1764
01765	FM	026000	001166	104.	0082.	FM	801.	0010.	0.	0000.	16/3 /240	1013	1765
01766	ST	060100	002327	104.	0083.	ST	600.	0014.	0.	0000.		1014	1766
01767	LQ	056000	002322	104.	0084.	LQ	600.	0009.	0.	0000.	1-BC/A	1015	1767
01770	FM	026000	001160	104.	0085.	FM	801.	0004.	0.	0000.	1/12	1016	1770
01771	FA	030000	001165	104.	0086.	FA	801.	0009.	0.	0000.	1/4	1017	1771
01772	LR	076500	000043	104.	0087.	LR	0.	0035.	0.	0000.		1018	1772
01773	FM	026000	002324	104.	0088.	FM	600.	0011.	0.	0000.		1019	1773
01774	CHS	076000	000002	104.	0089.	CHS	0.	0000.	0.	0000.		1020	1774
01775	FA	030000	001163	104.	0090.	FA	801.	0007.	0.	0000.	3/2	1021	1775
01776	FS	030200	002327	104.	0091.	FS	600.	0014.	0.	0000.		1022	1776
01777	LR	076500	000043	104.	0092.	LR	0.	0035.	0.	0000.		1023	1777
02000	FM	026000	001130	104.	0093.	FM	800.	0000.	0.	0000.	R	1024	2000
02001	ST	060100	002331	104.	0094.	ST	600.	0016.	0.	0000.	H/T ROT	1025	2001
02002	CA	050000	002327	104.	0095.	CA	600.	0014.	0.	0000.		1026	2002
02003	FA	030000	001163	104.	0096.	FA	801.	0007.	0.	0000.	3/2	1027	2003
02004	LR	076500	000043	104.	0097.	LR	0.	0035.	0.	0000.		1028	2004
02005	FM	026000	001130	104.	0098.	FM	800.	0000.	0.	0000.	R	1029	2005
02006	ST	060100	002333	104.	0099.	ST	600.	0018.	0.	0000.	C SUB P ROT	1030	2006
02007	CA	050000	002331	104.	0100.	CA	600.	0016.	0.	0000.	H/T	1031	2007
02010	FA	030000	002330	104.	0101.	FA	600.	0015.	0.	0000.	-F/T	1032	2010
02011	ST	060100	002332	104.	0102.	ST	600.	0017.	0.	0000.	S ROT	1033	2011
02012	FA	030000	000740	104.	0103.	FA	1.	0032.	0.	0000.	S TOT	1034	2012
02013	ST	060100	000740	104.	0103.1	ST	1.	0032.	0.	0000.		1035	2013
02014	CA	050000	000736	104.	0104.	CA	1.	0030.	0.	0000.		1036	2014
02015	FA	030000	002330	104.	0105.	FA	600.	0015.	0.	0000.	-F/T TOTAL	1037	2015
02016	ST	060100	000736	104.	0106.	ST	1.	0030.	0.	0000.		1038	2016
02017	CA	050000	000737	104.	0107.	CA	1.	0031.	0.	0000.		1039	2017

02020	FA	030000	002331	104.	0108.	FA	600.	0016.	0.	0000.		1040	2020
02021	ST	060100	000737	104.	0109.	ST	1.	0031.	0.	0000.	H/T TOTAL	1041	2021
02022	CA	050000	000741	104.	0110.	CA	1.	0033.	0.	0000.		1042	2022
02023	FA	030000	002333	104.	0111.	FA	600.	0018.	0.	0000.		1043	2023
02024	ST	060100	000741	104.	0112.	ST	1.	0033.	0.	0000.	C SUB P TOT	1044	2024
02025	CA	050000	000735	104.	0113.	CA	1.	0029.	0.	0000.		1045	2025
02026	ST	060100	002334	104.	0113.1	ST	600.	0019.	0.	0000.		1046	2026
02027	SE	076000	000161	104.	0114.	SE	0.	0113.	0.	0000.	SS NO. 1	1047	2027
02030	T	002000	002203	104.	0115.	T	106.	0000.	0.	0000.	PRINT	1048	2030
02031	T	002000	004420	104.	0116.	T	108.	0000.	0.	0000.	CALC STRETCH CORR.	1049	2031

02044	LQ	056000	001143	105.	0000.	LQ	800.	0011.	0.	0000.	HC/K	1060	2044	
02045	FM	026000	001217	105.	0001.	FM	802.	0005.	0.	0000.	B	1061	2045	
02046	FD	024000	000735	105.	0002.	FD	1.	0029.	0.	0000.	T	1062	2046	
02047	SQ	-060000	002311	105.	0003.	SQ	600.	0000.	0.	0000.	HCB/KT	1063	2047	
02050	CA	050000	001155	105.	0004.	CA	801.	0001.	0.	0000.	ONE	1064	2050	
02051	FD	024000	002311	105.	0005.	FD	600.	0000.	0.	0000.		1065	2051	
02052	SQ	-060000	002312	105.	0006.	SQ	600.	0001.	0.	0000.	KT/HCB	1066	2052	
02053	LQ	056000	002311	105.	0007.	LQ	600.	0000.	0.	0000.	HCB/KT	1067	2053	
02054	FM	026000	002311	105.	0008.	FM	600.	0000.	0.	0000.	SQ	1068	2054	
02055	ST	060100	002313	105.	0009.	ST	600.	0002.	0.	0000.		1069	2055	
02056	LQ	056000	002313	105.	0010.	LQ	600.	0002.	0.	0000.		1070	2056	
02057	FM	026000	002311	105.	0011.	FM	600.	0000.	0.	0000.	CUBED	1071	2057	
02060	ST	060100	002314	105.	0012.	ST	600.	0003.	0.	0000.		1072	2060	
02061	FD	024000	001173	105.	0013.	FD	801.	0015.	0.	0000.	315	1073	2061	
02062	SQ	-060000	002315	105.	0014.	SQ	600.	0004.	0.	0000.		1074	2062	
02063	CA	050000	002313	105.	0015.	CA	600.	0002.	0.	0000.		1075	2063	
02064	FD	024000	001173	105.	0016.	FD	801.	0015.	0.	0000.		1076	2064	
02065	FM	026000	001157	105.	0017.	FM	801.	0003.	0.	0000.	4	1077	2065	
02066	FA	030000	002315	105.	0018.	FA	600.	0004.	0.	0000.		1078	2066	
02067	FA	030000	001167	105.	0019.	FA	801.	0011.	0.	0000.	1/3	1079	2067	
02070	ST	060100	002315	105.	0020.	ST	600.	0004.	0.	0000.		1080	2070	
02071	LQ	056000	002311	105.	0021.	LQ	600.	0000.	0.	0000.		1081	2071	
02072	FM	026000	001174	105.	0022.	FM	801.	0016.	0.	0000.	1/15	1082	2072	
02073	FA	030000	002315	105.	0023.	FA	600.	0004.	0.	0000.		1083	2073	
02074	FA	030000	002312	105.	0024.	FA	600.	0001.	0.	0000.	KT/HCB	1084	2074	
02075	FD	024000	001214	105.	0025.	FD	802.	0002.	0.	0000.	SIGMA	1085	2075	
02076	SQ	-060000	002316	105.	0026.	SQ	600.	0005.	0.	0000.	Q	1086	2076	
02077	CA	050000	002316	105.	0027.	CA	600.	0005.	0.	0000.		1087	2077	
02100	TSX	007400	402373	105.	0028.	TSX	702.	0000.	C	0.	0000.	LN	1088	2100
02101	H	000000	000000	105.	0029.	H	0.	0000.	0.	0000.		1089	2101	
02102	LR	076500	000043	105.	0030.	LR	0.	0035.	0.	0000.		1090	2102	
02103	FM	026000	001130	105.	0031.	FM	800.	0000.	0.	0000.	R	1091	2103	
02104	ST	060100	002330	105.	0032.	ST	600.	0015.	0.	0000.	-F/T ROT	1092	2104	
02105	LQ	056000	002314	105.	0033.	LQ	600.	0003.	0.	0000.		1093	2105	
02106	FM	026000	001171	105.	0034.	FM	801.	0013.	0.	0000.	2.67/63	1094	2106	
02107	ST	060100	002317	105.	0035.	ST	600.	0006.	0.	0000.		1095	2107	
02110	LQ	056000	002313	105.	0036.	LQ	600.	0002.	0.	0000.		1096	2110	
02111	FM	026000	001170	105.	0037.	FM	801.	0012.	0.	0000.	1/9	1097	2111	
02112	ST	060100	002320	105.	0038.	ST	600.	0007.	0.	0000.		1098	2112	
02113	LQ	056000	002311	105.	0039.	LQ	600.	0000.	0.	0000.		1099	2113	
02114	FM	026000	001167	105.	0040.	FM	801.	0011.	0.	0000.	1/3	1100	2114	
02115	CHS	076000	000002	105.	0041.	CHS	0.	0000.	0.	0000.		1101	2115	
02116	FA	030000	001155	105.	0042.	FA	801.	0001.	0.	0000.	ONE	1102	2116	
02117	FS	030200	002317	105.	0043.	FS	600.	0006.	0.	0000.		1103	2117	

02120	FS	030200	002320	105.	0044.	FS	600.	0007.	0.	0000.		1104	2120	
02121	LR	076500	000043	105.	0045.	LR	0.	0035.	0.	0000.		1105	2121	
02122	FM	026000	001130	105.	0046.	FM	800.	0000.	0.	0000.	R	1106	2122	
02123	ST	060100	002331	105.	0047.	ST	600.	0016.	0.	0000.	H/T ROT	1107	2123	
02124	FA	030000	002330	105.	0048.	FA	600.	0015.	0.	0000.	-F/T ROT	1108	2124	
02125	ST	060100	002332	105.	0049.	ST	600.	0017.	0.	0000.	S ROT	1109	2125	
02126	LQ	056000	002314	105.	0050.	LQ	600.	0003.	0.	0000.		1110	2126	
02127	FM	026000	001171	105.	0051.	FM	801.	0013.	0.	0000.	2.67/63	1111	2127	
02130	LR	076500	000043	105.	0052.	LR	0.	0035.	0.	0000.		1112	2130	
02131	FM	026000	001156	105.	0053.	FM	801.	0002.	0.	0000.	TWO	1113	2131	
02132	ST	060100	002321	105.	0054.	ST	600.	0008.	0.	0000.		1114	2132	
02133	LQ	056000	002313	105.	0055.	LQ	600.	0002.	0.	0000.		1115	2133	
02134	FM	026000	001170	105.	0056.	FM	801.	0012.	0.	0000.	1/12	1116	2134	
02135	FA	030000	001155	105.	0057.	FA	801.	0001.	0.	0000.	ONE	1117	2135	
02136	FA	030000	002321	105.	0058.	FA	600.	0008.	0.	0000.		1118	2136	
02137	LR	076500	000043	105.	0059.	LR	0.	0035.	0.	0000.		1119	2137	
02140	FM	026000	001130	105.	0060.	FM	800.	0000.	0.	0000.	R	1120	2140	
02141	ST	060100	002333	105.	0061.	ST	600.	0018.	0.	0000.	C SUB P ROT	1121	2141	
02142	FA	030000	000741	105.	0062.	FA	1.	0033.	0.	0000.		1122	2142	
02143	ST	060100	000741	105.	0063.	ST	1.	0033.	0.	0000.	C SUB P TOT	1123	2143	
02144	CA	050000	002330	105.	0064.	CA	600.	0015.	0.	0000.		1124	2144	
02145	FA	030000	000736	105.	0065.	FA	1.	0030.	0.	0000.		1125	2145	
02146	ST	060100	000736	105.	0066.	ST	1.	0030.	0.	0000.	-F/T TOT	1126	2146	
02147	CA	050000	002331	105.	0067.	CA	600.	0016.	0.	0000.		1127	2147	
02150	FA	030000	000737	105.	0068.	FA	1.	0031.	0.	0000.		1128	2150	
02151	ST	060100	000737	105.	0069.	ST	1.	0031.	0.	0000.	H/T TOT	1129	2151	
02152	CA	050000	002332	105.	0070.	CA	600.	0017.	0.	0000.		1130	2152	
02153	FA	030000	000740	105.	0071.	FA	1.	0032.	0.	0000.		1131	2153	
02154	ST	060100	000740	105.	0072.	ST	1.	0032.	0.	0000.	S TOT	1132	2154	
02155	CA	050000	000735	105.	0073.	CA	1.	0029.	0.	0000.		1133	2155	
02156	ST	060100	002334	105.	0074.	ST	600.	0019.	0.	0000.		1134	2156	
02157	SE	076000	000161	105.	0075.	SE	0.	0113.	0.	0000.	SS NO. 1	1135	2157	
02160	T	002000	002203	105.	0076.	T	106.	0000.	0.	0000.	PRINT	1136	2160	
02161	T	002000	004420	105.	0077.	T	108.	0000.	0.	0000.	CALC STRETCH CORR.	1137	2161	
02203	CA	050000	000736	106.	0000.	CA	1.	0030.	0.	0000.	FREE ENERGY	1155	2203	
02204	ST	060100	002223	106.	0001.	ST	2.	0016.	0.	0000.		1156	2204	
02205	CA	050000	000737	106.	0002.	CA	1.	0031.	0.	0000.	ENTHALPY	1157	2205	
02206	ST	060100	002224	106.	0003.	ST	2.	0017.	0.	0000.		1158	2206	
02207	CA	050000	000740	106.	0004.	CA	1.	0032.	0.	0000.	ENTROPY	1159	2207	
02210	ST	060100	002225	106.	0005.	ST	2.	0018.	0.	0000.		1160	2210	
02211	CA	050000	000741	106.	0006.	CA	1.	0033.	0.	0000.	HEAT CAPACITY	1161	2211	
02212	ST	060100	002226	106.	0007.	ST	2.	0019.	0.	0000.		1162	2212	
02213	TSX	007400	402450	106.	0008.	TSX	703.	0000.	C	0.	0000.	LAS 117 Fxd PT PRINT	1163	2213
02214	SIX	-203744	002334	106.	0009.	SIX	600.	0019.	0.	2020.	TEMP	1164	2214	
02215	SIX	-211660	002223	106.	0010.	SIX	2.	0016.	0.	5040.		1165	2215	
02216	SIX	-211794	002224	106.	0011.	SIX	2.	0017.	0.	5060.		1166	2216	
02217	SIX	-211730	002225	106.	0012.	SIX	2.	0018.	0.	5080.		1167	2217	
02220	SIX	-211754	002226	106.	0013.	SIX	2.	0019.	0.	5100.		1168	2220	
02221	PON	100000	000000	106.	0014.	PON	0.	0000.	0.	0000.		1169	2221	
02222	T	002000	002241	106.	0015.	T	107.	0000.	0.	0000.	INCREMENT TEMP	1170	2222	
02223	H	000000	000000	106.	0016.	H	0.	0000.	0.	0000.		1171	2223	
02224	H	000000	000000	106.	0017.	H	0.	0000.	0.	0000.		1172	2224	
02225	H	000000	000000	106.	0018.	H	0.	0000.	0.	0000.		1173	2225	
02226	H	000000	000000	106.	0019.	H	0.	0000.	0.	0000.		1174	2226	
02227	SDX	-053400	402236	106.	0021.	SDX	2.	0028.	C	0.	0000.		1175	2227
02230	ZS	060000	406117	106.	0022.	ZS	804.	0011.	C	0.	0000.	DELTA S	1176	2230

02231 TX	200001	402230	106. 0023.	TX	2. 0022.	C	0. 0001.	1177	2231
02232 SDX	-053400	402237	106. 0024.	SDX	2. 0029.	C	0. 0000.	1178	2232
02233 ZS	060000	406212	106. 0025.	ZS	805. 0055.	C	0. 0000.	1179	2233
02234 TX	200001	402233	106. 0026.	TX	2. 0025.	C	0. 0001.	1180	2234
02235 T	002000	002304	106. 0027.	T	107. 0029.		0. 0000.	1181	2235
02236	000013	000000	106. 0028.		0. 0000.		0. 0011.	1182	2236
02237	000067	000000	106. 0029.		0. 0000.		0. 0055.	1183	2237
								ANHARMONICITIES	
								READ IN NEW DATA	
02241 CA	050000	002334	107. 0000.	CA	600. 0019.		0. 0000.	1185	2241
02242 FS	030200	001366	107. 0001.	FS	803. 0008.		0. 0000.	1186	2242
02243 TM	-012000	002261	107. 0002.	TM	2. 0016.		0. 0000.	1187	2243
02244 CA	050000	002334	107. 0003.	CA	600. 0019.		0. 0000.	1188	2244
02245 FS	030200	001360	107. 0004.	FS	803. 0002.		0. 0000.	1189	2245
02246 TM	-012000	002265	107. 0005.	TM	2. 0020.		0. 0000.	1190	2246
02247 CA	050000	002334	107. 0006.	CA	600. 0019.		0. 0000.	1191	2247
02250 FS	030200	001360	107. 0007.	FS	803. 0002.		0. 0000.	1192	2250
02251 TZ	010000	002270	107. 0008.	TZ	2. 0023.		0. 0000.	1193	2251
02252 CA	050000	002334	107. 0009.	CA	600. 0019.		0. 0000.	1194	2252
02253 FA	030000	001362	107. 0010.	FA	803. 0004.		0. 0000.	1195	2253
02254 ST	060100	000735	107. 0011.	ST	1. 0029.		0. 0000.	1196	2254
02255 FS	030200	001364	107. 0012.	FS	803. 0006.		0. 0000.	1197	2255
02256 TP	012000	002273	107. 0013.	TP	2. 0026.		0. 0000.	1198	2256
02257 CA	050000	000735	107. 0014.	CA	1. 0029.		0. 0000.	1199	2257
02260 T	002000	001466	107. 0015.	T	102. 0002.		0. 0000.	1200	2260
02261 CA	050000	002334	107. 0016.	CA	600. 0019.		0. 0000.	1201	2261
02262 FA	030000	001357	107. 0017.	FA	803. 0001.		0. 0000.	1202	2262
02263 ST	060100	000735	107. 0018.	ST	1. 0029.		0. 0000.	1203	2263
02264 T	002000	001466	107. 0019.	T	102. 0002.		0. 0000.	1204	2264
02265 CA	050000	001360	107. 0020.	CA	803. 0002.		0. 0000.	1205	2265
02266 ST	060100	000735	107. 0021.	ST	1. 0029.		0. 0000.	1206	2266
02267 T	002000	001466	107. 0022.	T	102. 0002.		0. 0000.	1207	2267
02270 CA	050000	001361	107. 0023.	CA	803. 0003.		0. 0000.	1208	2270
02271 ST	060100	000735	107. 0024.	ST	1. 0029.		0. 0000.	1209	2271
02272 T	002000	001466	107. 0025.	T	102. 0002.		0. 0000.	1210	2272
02273 RD	076200	000361	107. 0026.	RD	0. 0241.		0. 0000.	1211	2273
02274 SE	076000	000370	107. 0027.	SE	0. 0248.		0. 0000.	1212	2274
02275 HP	042000	000000	107. 0027.1	HP	0. 0000.		0. 0000.	1213	2275
02276 SDX	-053400	402305	107. 0027.2	SDX	2. 0030.	C	0. 0000.	1214	2276
02277 ZS	060000	401315	107. 0027.3	ZS	802. 0067.	C	0. 0000.	1215	2277
02300 TX	200001	402277	107. 0027.4	TX	2. 0027.3	C	0. 0001.	1216	2300
02301 TSX	007400	403422	107. 0028.	TSX	706. 0000.	C	0. 0000.	1217	2301
02302 ZS	060000	002320	107. 0028.1	ZS	600. 0007.		0. 0000.	1218	2302
02303 T	002000	002227	107. 0028.2	T	106. 0021.		0. 0000.	1219	2303
02304 T	002000	003472	107. 0029.	T	707. 0010.		0. 0000.	1220	2304
02305	000103	000000	107. 0030.		0. 0000.		0. 0067.	1221	2305
								TEMPORARY T	
								250 DEG	
								T LESS 250	
								298.16	
								T EQUAL 250	
								T EQUAL 298	
								INC T BY 100	
								5010 DEG	
								RECYCLE	
								T WKG	
								INC T BY 50	
								RECYCLE	
								298.16	
								RECYCLE	
								300	
								RECYCLE	
								SKIP PAGE	
								END OF PROBLEM	
								BINARY LD	
								STORE ZEROS	
								DEC LD	

04420	LQ	056000	000735	108.	0000.	LQ	1.	0029.	0.	0000.	T	2320	4420
04421	FM	026000	006104	108.	0001.	FM	804.	0000.	0.	0000.	RHO	2321	4421
04422	FA	030000	001155	108.	0002.	FA	801.	0001.	0.	0000.	1	2322	4422
04423	ST	060100	005233	108.	0003.	ST	602.	0000.	0.	0000.	Q STRETCH	2323	4423
04424	TSX	007400	402373	108.	0004.	TSX	702.	0000.	C	0.	LN	2324	4424
04425	ZS	060000	005234	108.	0005.	ZS	602.	0001.	0.	0000.	OF ZERO	2325	4425
04426	ST	060100	005234	108.	0006.	ST	602.	0001.	0.	0000.		2326	4426
04427	LR	076500	000043	108.	0006.1	LR	0.	0035.	0.	0000.		2327	4427
04430	FM	026000	001130	108.	0006.2	FM	800.	0000.	0.	0000.	R	2328	4430
04431	ST	060100	005234	108.	0006.3	ST	602.	0001.	0.	0000.	-F/T STRETCH	2329	4431
04432	FA	030000	000736	108.	0007.	FA	1.	0030.	0.	0000.		2330	4432
04433	ST	060100	000736	108.	0008.	ST	1.	0030.	0.	0000.	-F/T TOTAL	2331	4433
04434	LQ	056000	006104	108.	0009.	LQ	804.	0000.	0.	0000.	RHO	2332	4434
04435	FM	026000	000735	108.	0010.	FM	1.	0029.	0.	0000.	T	2333	4435
04436	LR	076500	000043	108.	0011.	LR	0.	0035.	0.	0000.		2334	4436
04437	FM	026000	001130	108.	0012.	FM	800.	0000.	0.	0000.	R	2335	4437
04440	ST	060100	005235	108.	0013.	ST	602.	0002.	0.	0000.	RTRHO	2336	4440
04441	FD	024000	005233	108.	0014.	FD	602.	0000.	0.	0000.		2337	4441
04442	SQ	-060000	005236	108.	0015.	SQ	602.	0003.	0.	0000.	H/T	2338	4442
04443	CA	050000	005236	108.	0016.	CA	602.	0003.	0.	0000.		2339	4443
04444	FA	030000	005234	108.	0017.	FA	602.	0001.	0.	0000.	-F/T	2340	4444
04445	FA	030000	000740	108.	0018.	FA	1.	0032.	0.	0000.		2341	4445
04446	ST	060100	000740	108.	0019.	ST	1.	0032.	0.	0000.	S TOTAL	2342	4446
04447	CA	050000	005236	108.	0020.	CA	602.	0003.	0.	0000.		2343	4447
04450	FA	030000	000737	108.	0021.	FA	1.	0031.	0.	0000.		2344	4450
04451	ST	060100	000737	108.	0022.	ST	1.	0031.	0.	0000.	H/T TOTAL	2345	4451
04452	LQ	056000	005236	108.	0023.	LQ	602.	0003.	0.	0000.		2346	4452
04453	FM	026000	001156	108.	0024.	FM	801.	0002.	0.	0000.	2	2347	4453
04454	ST	060100	005237	108.	0025.	ST	602.	0004.	0.	0000.		2348	4454
04455	LQ	056000	005236	108.	0026.	LQ	602.	0003.	0.	0000.		2349	4455
04456	FM	026000	005236	108.	0027.	FM	602.	0003.	0.	0000.		2350	4456
04457	FD	024000	001130	108.	0028.	FD	800.	0000.	0.	0000.	R	2351	4457
04460	SQ	-060000	005240	108.	0029.	SQ	602.	0005.	0.	0000.		2352	4460
04461	CS	050200	005240	108.	0030.	CS	602.	0005.	0.	0000.		2353	4461
04462	FA	030000	005237	108.	0031.	FA	602.	0004.	0.	0000.		2354	4462
04463	ST	060100	005237	108.	0032.	ST	602.	0004.	0.	0000.	C SUB P STRETCH	2355	4463
04464	FA	030000	000741	108.	0033.	FA	1.	0033.	0.	0000.		2356	4464
04465	ST	060100	000741	108.	0034.	ST	1.	0033.	0.	0000.	C SUB P TOTAL	2357	4465
04466	T	002000	004475	108.	0035.	T	109.	0000.	0.	0000.	CALC V1B-ROT INTERACT	2358	4466
04475	SDX	-053400	204652	109.	0000.	SDX	2.	0104.	B	0.		2365	4475
04476	SDX	-053400	104653	109.	0001.	SDX	2.	0105.	A	0.		2366	4476
04477	CA	050000	201304	109.	0002.	CA	802.	0058.	B	0.	G SUB EYE	2367	4477
04500	TZ	010000	004711	109.	0003.	TZ	110.	0000.		0.	PAST LAST NU	2368	4500
04501	LQ	056000	001143	109.	0004.	LQ	800.	0011.		0.	HC/K	2369	4501
04502	FM	026000	201303	109.	0005.	FM	802.	0057.	B	0.	NU SUB EYE	2370	4502
04503	FD	024000	000735	109.	0006.	FD	1.	0029.		0.	T	2371	4503
04504	SQ	-060000	005245	109.	0007.	SQ	603.	0000.		0.	U SUB EYE	2372	4504
04505	CA	050000	005245	109.	0008.	CA	603.	0000.		0.		2373	4505
04506	TSX	007400	403314	109.	0009.	TSX	704.	0000.	C	0.	EXPON	2374	4506
04507	T	002000	004654	109.	0010.	T	2.	0106.		0.	GREATER THAN 87	2375	4507
04510	ST	060100	005246	109.	0011.	ST	603.	0001.		0.		2376	4510
04511	FS	030200	001155	109.	0012.	FS	801.	0001.		0.	1	2377	4511

04512	ST	060100	005247	109.	0013.	ST	603.	0002.	0.	0000.	E TO U -1	2378	4512
04513	TZ	010000	004711	109.	0013.1	TZ	110.	0000.	0.	0000.	CALC ANHARM FNS	2379	4513
04514	LQ	056000	005247	109.	0014.	LQ	603.	0002.	0.	0000.		2380	4514
04515	FM	026000	005247	109.	0015.	FM	603.	0002.	0.	0000.	SQ	2381	4515
04516	TF	014000	004657	109.	0015.1	TF	2.	0109.	0.	0000.		2382	4516
04517	ST	060100	005250	109.	0016.	ST	603.	0003.	0.	0000.		2383	4517
04520	LQ	056000	106117	109.	0017.	LQ	804.	0011.	A	0.0000.	DELTA SUB EYE	2384	4520
04521	FM	026000	201304	109.	0018.	FM	802.	0058.	B	0.0000.	G	2385	4521
04522	FD	024000	005247	109.	0019.	FD	603.	0002.		0.0000.		2386	4522
04523	SQ	-060000	005251	109.	0020.	SQ	603.	0004.		0.0000.		2387	4523
04524	CA	050000	005251	109.	0021.	CA	603.	0004.		0.0000.		2388	4524
04525	FA	030000	001155	109.	0022.	FA	801.	0001.		0.0000.	1	2389	4525
04526	ST	060100	005252	109.	0023.	ST	603.	0005.		0.0000.		2390	4526
04527	TSX	007400	402373	109.	0024.	TSX	702.	0000.	C	0.0000.	LN	2391	4527
04530	HP	042000	000000	109.	0025.	HP	0.	0000.		0.0000.		2392	4530
04531	LR	076500	000043	109.	0026.	LR	0.	0035.		0.0000.		2393	4531
04532	FM	026000	001130	109.	0027.	FM	800.	0000.		0.0000.	R	2394	4532
04533	ST	060100	005253	109.	0028.	ST	603.	0006.		0.0000.	-F/T,V-R	2395	4533
04534	FA	030000	000736	109.	0029.	FA	1.	0030.		0.0000.		2396	4534
04535	ST	060100	000736	109.	0030.	ST	1.	0030.		0.0000.	-F/T,TOTAL	2397	4535
04536	LQ	056000	001143	109.	0031.	LQ	800.	0011.		0.0000.	HC/K	2398	4536
04537	FM	026000	201303	109.	0032.	FM	802.	0057.	B	0.0000.	NU	2399	4537
04540	LR	076500	000043	109.	0033.	LR	0.	0035.		0.0000.		2400	4540
04541	FM	026000	106117	109.	0034.	FM	804.	0011.	A	0.0000.	DELTA	2401	4541
04542	LR	076500	000043	109.	0035.	LR	0.	0035.		0.0000.		2402	4542
04543	FM	026000	201304	109.	0036.	FM	802.	0058.	B	0.0000.	G	2403	4543
04544	LR	076500	000043	109.	0037.	LR	0.	0035.		0.0000.		2404	4544
04545	FM	026000	005246	109.	0038.	FM	603.	0001.		0.0000.	E TO U	2405	4545
04546	TF	014000	004661	109.	0038.1	TF	2.	0111.		0.0000.		2406	4546
04547	ST	060100	005254	109.	0039.	ST	603.	0007.		0.0000.		2407	4547
04550	LQ	056000	106117	109.	0040.	LQ	804.	0011.	A	0.0000.	DELTA	2408	4550
04551	FM	026000	201304	109.	0041.	FM	802.	0058.	B	0.0000.	G	2409	4551
04552	FS	030200	001155	109.	0042.	FS	801.	0001.		0.0000.	1	2410	4552
04553	FA	030000	005246	109.	0043.	FA	603.	0001.		0.0000.		2411	4553
04554	ST	060100	005255	109.	0044.	ST	603.	0008.		0.0000.		2412	4554
04555	LQ	056000	001143	109.	0045.	LQ	800.	0011.		0.0000.		2413	4555
04556	FM	026000	201303	109.	0046.	FM	802.	0057.	B	0.0000.	NU	2414	4556
04557	ST	060100	005256	109.	0047.	ST	603.	0009.		0.0000.	HC NU/K	2415	4557
04560	CA	050000	005254	109.	0048.	CA	603.	0007.		0.0000.		2416	4560
04561	FD	024000	005247	109.	0049.	FD	603.	0002.		0.0000.	E TO U -1	2417	4561
04562	FM	026000	001130	109.	0050.	FM	800.	0000.		0.0000.	R	2418	4562
04563	FD	024000	005255	109.	0051.	FD	603.	0008.		0.0000.		2419	4563
04564	SQ	-060000	005257	109.	0052.	SQ	603.	0010.		0.0000.		2420	4564
04565	CA	050000	005257	109.	0053.	CA	603.	0010.		0.0000.		2421	4565
04566	FD	024000	000735	109.	0054.	FD	1.	0029.		0.0000.	T	2422	4566
04567	SQ	-060000	005257	109.	0055.	SQ	603.	0010.		0.0000.	H/T,V-R	2423	4567
04570	CA	050000	005257	109.	0056.	CA	603.	0010.		0.0000.		2424	4570
04571	FA	030000	005253	109.	0057.	FA	603.	0006.		0.0000.	-F/T,V-R	2425	4571
04572	FA	030000	000740	109.	0058.	FA	1.	0032.		0.0000.		2426	4572
04573	ST	060100	000740	109.	0059.	ST	1.	0032.		0.0000.	S,TOTAL	2427	4573
04574	CA	050000	005257	109.	0060.	CA	603.	0010.		0.0000.		2428	4574
04575	FA	030000	000737	109.	0061.	FA	1.	0031.		0.0000.		2429	4575
04576	ST	060100	000737	109.	0062.	ST	1.	0031.		0.0000.	H/T,TOTAL	2430	4576

04577	LQ	056000	005257	109.	0063.	LQ	603.	0010.	0.	0000.		2431	4577
04600	FM	026000	005257	109.	0064.	FM	603.	0010.	0.	0000.		2432	4600
04601	FD	024000	001130	109.	0065.	FD	800.	0000.	0.	0000.	R	2433	4601
04602	SQ	-060000	005260	109.	0066.	SQ	603.	0011.	0.	0000.		2434	4602
04603	LQ	056000	005254	109.	0067.	LQ	603.	0007.	0.	0000.		2435	4603
04604	FM	026000	001156	109.	0068.	FM	801.	0002.	0.	0000.	2	2436	4604
04605	LR	076500	000043	109.	0069.	LR	0.	0035.	0.	0000.		2437	4605
04606	FM	026000	005247	109.	0070.	FM	603.	0002.	0.	0000.	E TO U -1	2438	4606
04607	TF	014000	004663	109.	0070.1	TF	2.	0113.	0.	0000.		2439	4607
04610	LR	076500	000043	109.	0071.	LR	0.	0035.	0.	0000.		2440	4610
04611	FM	026000	005256	109.	0072.	FM	603.	0009.	0.	0000.	HC NU/K	2441	4611
04612	LR	076500	000043	109.	0073.	LR	0.	0035.	0.	0000.		2442	4612
04613	FM	026000	005246	109.	0074.	FM	603.	0001.	0.	0000.	E TO U	2443	4613
04614	TF	014000	004665	109.	0074.1	TF	2.	0115.	0.	0000.		2444	4614
04615	ST	060100	005261	109.	0075.	ST	603.	0012.	0.	0000.		2445	4615
04616	LQ	056000	005250	109.	0076.	LQ	603.	0003.	0.	0000.	E TO U -1 SQ	2446	4616
04617	FM	026000	005254	109.	0077.	FM	603.	0007.	0.	0000.		2447	4617
04620	TF	014000	004667	109.	0077.1	TF	2.	0117.	0.	0000.		2448	4620
04621	LR	076500	000043	109.	0078.	LR	0.	0035.	0.	0000.		2449	4621
04622	FM	026000	005256	109.	0079.	FM	603.	0009.	0.	0000.	HC NU/K	2450	4622
04623	CHS	076000	000002	109.	0080.	CHS	0.	0000.	0.	0000.		2451	4623
04624	FA	030000	005261	109.	0081.	FA	603.	0012.	0.	0000.		2452	4624
04625	FD	024000	005250	109.	0082.	FD	603.	0003.	0.	0000.		2453	4625
04626	FM	026000	001130	109.	0083.	FM	800.	0000.	0.	0000.	R	2454	4626
04627	FD	024000	005247	109.	0084.	FD	603.	0002.	0.	0000.	E TO U -1	2455	4627
04630	SQ	-060000	005262	109.	0085.	SQ	603.	0013.	0.	0000.		2456	4630
04631	CA	050000	005262	109.	0086.	CA	603.	0013.	0.	0000.		2457	4631
04632	FD	024000	005255	109.	0087.	FD	603.	0008.	0.	0000.		2458	4632
04633	SQ	-060000	005262	109.	0088.	SQ	603.	0013.	0.	0000.		2459	4633
04634	CA	050000	005262	109.	0089.	CA	603.	0013.	0.	0000.		2460	4634
04635	FD	024000	000735	109.	0090.	FD	1.	0029.	0.	0000.	T	2461	4635
04636	SQ	-060000	005262	109.	0091.	SQ	603.	0013.	0.	0000.		2462	4636
04637	CA	050000	005262	109.	0092.	CA	603.	0013.	0.	0000.		2463	4637
04640	FD	024000	000735	109.	0093.	FD	1.	0029.	0.	0000.	T	2464	4640
04641	SQ	-060000	005262	109.	0094.	SQ	603.	0013.	0.	0000.		2465	4641
04642	CA	050000	005262	109.	0098.	CA	603.	0013.	0.	0000.		2466	4642
04643	FS	030200	005260	109.	0099.	FS	603.	0011.	0.	0000.		2467	4643
04644	ST	060100	005263	109.	0100.	ST	603.	0014.	0.	0000.	C SUB P, B-R	2468	4644
04645	FA	030000	000741	109.	0101.	FA	1.	0033.	0.	0000.		2469	4645
04646	ST	060100	000741	109.	0102.	ST	1.	0033.	0.	0000.	C SUB P, TOTAL	2470	4646
04647	TX	200001	104650	109.	0102.1	TX	2.	0102.2	0.	0001.	A	2471	4647
04650	TX	200002	204477	109.	0102.2	TX	2.	0002.	0.	0002.	B	2472	4650
04651	T	002000	004711	109.	0103.	T	110.	0000.	0.	0000.		2473	4651
04652		000062	000000	109.	0104.		0.	0000.	0.	0050.		2474	4652
04653		000012	000000	109.	0105.		0.	0000.	0.	0010.		2475	4653
04654	CA	050000	006227	109.	0106.	CA	806.	0003.	0.	0000.		2476	4654
04655	ST	060100	005246	109.	0107.	ST	603.	0001.	0.	0000.		2477	4655
04656	T	002000	004511	109.	0108.	T	2.	0012.	0.	0000.		2478	4656
04657	CA	050000	006227	109.	0109.	CA	806.	0003.	0.	0000.		2479	4657
04660	T	002000	004517	109.	0110.	T	2.	0016.	0.	0000.		2480	4660
04661	CA	050000	006227	109.	0111.	CA	806.	0003.	0.	0000.		2481	4661
04662	T	002000	004547	109.	0112.	T	2.	0039.	0.	0000.		2482	4662
04663	CA	050000	006227	109.	0113.	CA	806.	0003.	0.	0000.		2483	4663
04664	T	002000	004610	109.	0114.	T	2.	0071.	0.	0000.		2484	4664
04665	CA	050000	006227	109.	0115.	CA	806.	0003.	0.	0000.		2485	4665
04666	T	002000	004615	109.	0116.	T	2.	0075.	0.	0000.		2486	4666
04667	CA	050000	006227	109.	0117.	CA	806.	0003.	0.	0000.		2487	4667
04670	T	002000	004621	109.	0118.	T	2.	0078.	0.	0000.		2488	4670

04711	SDX	-053400	106224	110.	0000.	SDX	806.	0000.	A	0.	0000.	I	2505	4711
04712	SDX	-053400	206225	110.	0001.	SDX	806.	0001.	B	0.	0000.	NO. OF NU,S	2506	4712
04713	CA	050000	201303	110.	0002.	CA	802.	0057.	B	0.	0000.	NU SUB I	2507	4713
04714	FD	024000	000735	110.	0003.	FD	1.	0029.		0.	0000.	T	2508	4714
04715	FM	026000	001143	110.	0004.	FM	800.	0011.		0.	0000.	HC/K	2509	4715
04716	TSX	007400	403314	110.	0005.	TSX	704.	0000.	C	0.	0000.	EXPON.	2510	4716
04717	T	002000	004771	110.	0006.	T	2.	0047.		0.	0000.	MORE THAN 87	2511	4717
04720	ST	060100	105303	110.	0007.	ST	604.	0010.	A	0.	0000.	E TO U	2512	4720
04721	FS	030200	001155	110.	0008.	FS	801.	0001.		0.	0000.	1	2513	4721
04722	ST	060100	105315	110.	0009.	ST	604.	0020.	A	0.	0000.	MINUS 1	2514	4722
04723	CA	050000	201304	110.	0010.	CA	802.	0058.	B	0.	0000.	G SUB I	2515	4723
04724	ST	060100	105327	110.	0011.	ST	604.	0030.	A	0.	0000.		2516	4724
04725	CA	050000	201303	110.	0012.	CA	802.	0057.	B	0.	0000.		2517	4725
04726	ST	060100	105341	110.	0013.	ST	604.	0040.	A	0.	0000.	NU SUB I	2518	4726
04727	TX	200002	204730	110.	0014.	TX	2.	0015.	B	0.	0002.		2519	4727
04730	TX	200001	104713	110.	0015.	TX	2.	0002.	A	0.	0001.		2520	4730
04731	SDX	-053400	106224	110.	0016.	SDX	806.	0000.	A	0.	0000.	I	2521	4731
04732	SDX	-053400	206224	110.	0017.	SDX	806.	0000.	B	0.	0000.	J	2522	4732
04733	SDX	-053400	406226	110.	0017.1	SDX	806.	0002.	C	0.	0000.	NO. OF X SUB IJ	2523	4733
04734	XAD	-075400	200000	110.	0018.	XAD	0.	0000.	B	0.	0000.		2524	4734
04735	ST	060100	005372	110.	0019.	ST	605.	0000.		0.	0000.		2525	4735
04736	XAD	-075400	100000	110.	0020.	XAD	0.	0000.	A	0.	0000.		2526	4736
04737	CAS	034000	005372	110.	0021.	CAS	605.	0000.		0.	0000.		2527	4737
04740	T	002000	004764	110.	0022.	T	2.	0043.		0.	0000.	I LESS THAN J	2528	4740
04741	T	002000	004743	110.	0023.	T	2.	0025.		0.	0000.	I EQUALS J	2529	4741
04742	TX	200001	204734	110.	0024.	TX	2.	0018.	B	0.	0001.	I MORE THAN J	2530	4742
04743	CA	050000	001155	110.	0025.	CA	801.	0001.		0.	0000.	1	2531	4743
04744	FA	030000	205327	110.	0026.	FA	604.	0030.	B	0.	0000.	G SUB J	2532	4744
04745	ST	060100	005373	110.	0027.	ST	605.	0001.		0.	0000.		2533	4745
04746	LQ	056000	005373	110.	0028.	LQ	605.	0001.		0.	0000.		2534	4746
04747	FM	026000	105327	110.	0029.	FM	604.	0030.	A	0.	0000.	G SUB I	2535	4747
04750	FD	024000	000735	110.	0030.	FD	1.	0029.		0.	0000.	T	2536	4750
04751	FM	026000	001143	110.	0031.	FM	800.	0011.		0.	0000.	HC/K	2537	4751
04752	ST	060100	005374	110.	0032.	ST	605.	0002.		0.	0000.		2538	4752
04753	LQ	056000	406212	110.	0034.	LQ	805.	0055.	C	0.	0000.	X SUB IJ	2539	4753
04754	FM	026000	005374	110.	0035.	FM	605.	0002.		0.	0000.		2540	4754
04755	ST	060100	406077	110.	0036.	ST	610.	0055.	C	0.	0000.	B SUB IJ	2541	4755
04756	LR	076500	000043	110.	0037.	LR	0.	0035.		0.	0000.		2542	4756
04757	FM	026000	000735	110.	0038.	FM	1.	0029.		0.	0000.	T	2543	4757
04760	ST	060100	405512	110.	0039.	ST	606.	0055.	C	0.	0000.	B PRIME IJ	2544	4760
04761	TX	200001	404762	110.	0040.	TX	2.	0041.	C	0.	0001.		2545	4761
04762	TX	200001	204734	110.	0041.	TX	2.	0018.	B	0.	0001.	INCREASE J BY ONE	2546	4762
04763	T	002000	004766	110.	0042.	T	2.	0045.		0.	0000.	J= J MAX	2547	4763
04764	CA	050000	001154	110.	0043.	CA	801.	0000.		0.	0000.	ZERO	2548	4764
04765	T	002000	004744	110.	0044.	T	2.	0026.		0.	0000.		2549	4765
04766	SDX	-053400	206224	110.	0045.	SDX	806.	0000.	B	0.	0000.		2550	4766
04767	TX	200001	104734	110.	0045.1	TX	2.	0018.	A	0.	0001.	INCREASE I BY ONE	2551	4767
04770	T	002000	004774	110.	0046.	T	2.	0050.		0.	0000.		2552	4770
04771	CA	050000	006227	110.	0047.	CA	806.	0003.		0.	0000.	10 TO THE 30	2553	4771
04772	ST	060100	105303	110.	0048.	ST	604.	0010.	A	0.	0000.		2554	4772
04773	T	002000	004721	110.	0049.	T	2.	0008.		0.	0000.		2555	4773
04774	SDX	-053400	106224	110.	0050.	SDX	806.	0000.	A	0.	0000.	I	2556	4774
04775	SDX	-053400	206224	110.	0051.	SDX	806.	0000.	B	0.	0000.	J	2557	4775
04776	SDX	-053400	406226	110.	0052.	SDX	806.	0002.	C	0.	0000.	NO. OF X SUB 1,J	2558	4776
04777	XAD	-075400	200000	110.	0053.	XAD	0.	0000.	B	0.	0000.		2559	4777

05067	FD	024000	205613	110.	0104.	FD	607.	0055.	B	0.	0000.	A	2615	5067
05070	SQ	-060000	005403	110.	0105.	SQ	605.	0009.		0.	0000.		2616	5070
05071	CA	050000	001155	110.	0106.	CA	801.	0001.		0.	0000.	1	2617	5071
05072	FA	030000	005403	110.	0107.	FA	605.	0009.		0.	0000.		2618	5072
05073	ST	060100	005403	110.	0108.	ST	605.	0009.		0.	0000.	1+B/A	2619	5073
05074	TSX	007400	402373	110.	0109.	TSX	702.	0000.	C	0.	0000.	LN	2620	5074
05075	HP	042000	000000	110.	0110.	HP	0.	0000.		0.	0000.	OF NEG NO.	2621	5075
05076	LR	076500	000043	110.	0111.	LR	0.	0035.		0.	0000.		2622	5076
05077	FM	026000	001130	110.	0112.	FM	800.	0000.		0.	0000.	R	2623	5077
05100	ST	060100	005404	110.	0113.	ST	605.	0010.		0.	0000.	-F/T, ANHARM	2624	5100
05101	FA	030000	000736	110.	0114.	FA	1.	0030.		0.	0000.		2625	5101
05102	ST	060100	000736	110.	0115.	ST	1.	0030.		0.	0000.		2626	5102
05103	LQ	056000	205707	110.	0116.	LQ	608.	0055.	B	0.	0000.	A PRIME	2627	5103
05104	FM	026000	206077	110.	0117.	FM	610.	0055.	B	0.	0000.	B	2628	5104
05105	ST	060100	005405	110.	0118.	ST	605.	0011.		0.	0000.		2629	5105
05106	LQ	056000	205512	110.	0119.	LQ	606.	0055.	B	0.	0000.	B PRIME	2630	5106
05107	FM	026000	205613	110.	0120.	FM	607.	0055.	B	0.	0000.	A	2631	5107
05110	FS	030200	005405	110.	0121.	FS	605.	0011.		0.	0000.		2632	5110
05111	ST	060100	005406	110.	0122.	ST	605.	0012.		0.	0000.		2633	5111
05112	FD	024000	205613	110.	0122.1	FD	607.	0055.	B	0.	0000.	A	2634	5112
05113	SQ	-060000	005407	110.	0122.2	SQ	605.	0013.		0.	0000.		2635	5113
05114	CA	050000	206077	110.	0123.	CA	610.	0055.	B	0.	0000.	B	2636	5114
05115	FA	030000	205613	110.	0124.	FA	607.	0055.	B	0.	0000.	A	2637	5115
05116	ST	060100	005406	110.	0125.	ST	605.	0012.		0.	0000.	A+B	2638	5116
05117	CS	050200	005407	110.	0126.	CS	605.	0013.		0.	0000.		2639	5117
05120	FD	024000	005406	110.	0127.	FD	605.	0012.		0.	0000.		2640	5120
05121	FM	026000	001130	110.	0130.	FM	800.	0000.		0.	0000.	R	2641	5121
05122	FD	024000	000735	110.	0131.	FD	1.	0029.		0.	0000.	T	2642	5122
05123	SQ	-060000	005410	110.	0132.	SQ	605.	0014.		0.	0000.	H/T ANHARM	2643	5123
05124	CA	050000	005410	110.	0133.	CA	605.	0014.		0.	0000.		2644	5124
05125	FA	030000	005404	110.	0134.	FA	605.	0010.		0.	0000.	-F/T	2645	5125
05126	FA	030000	000740	110.	0135.	FA	1.	0032.		0.	0000.		2646	5126
05127	ST	060100	000740	110.	0136.	ST	1.	0032.		0.	0000.	S, TOTAL	2647	5127
05130	CA	050000	005410	110.	0137.	CA	605.	0014.		0.	0000.		2648	5130
05131	FA	030000	000737	110.	0138.	FA	1.	0031.		0.	0000.		2649	5131
05132	ST	060100	000737	110.	0139.	ST	1.	0031.		0.	0000.	H/T, TOTAL	2650	5132
05133	LQ	056000	005410	110.	0140.	LQ	605.	0014.		0.	0000.		2651	5133
05134	FM	026000	005410	110.	0141.	FM	605.	0014.		0.	0000.		2652	5134
05135	FD	024000	001130	110.	0142.	FD	800.	0000.		0.	0000.	R	2653	5135
05136	SQ	-060000	005411	110.	0143.	SQ	605.	0015.		0.	0000.		2654	5136
05137	CS	050200	206003	110.	0144.	CS	609.	0055.	B	0.	0000.	A DUBL PRIME	2655	5137
05140	FD	024000	005406	110.	0145.	FD	605.	0012.		0.	0000.	A+B	2656	5140
05141	FM	026000	206077	110.	0146.	FM	610.	0055.	B	0.	0000.	B	2657	5141
05142	FD	024000	205613	110.	0147.	FD	607.	0055.	B	0.	0000.	A	2658	5142
05143	SQ	-060000	005412	110.	0148.	SQ	605.	0016.		0.	0000.		2659	5143
05144	CS	050200	205707	110.	0149.	CS	608.	0055.	B	0.	0000.	A PRIME	2660	5144
05145	FD	024000	005406	110.	0150.	FD	605.	0012.		0.	0000.	A+B	2661	5145
05146	FM	026000	205512	110.	0151.	FM	606.	0055.	B	0.	0000.	B PRIME	2662	5146
05147	FD	024000	205613	110.	0152.	FD	607.	0055.	B	0.	0000.	A	2663	5147
05150	FM	026000	001156	110.	0153.	FM	801.	0002.		0.	0000.	2	2664	5150
05151	FA	030000	005412	110.	0154.	FA	605.	0016.		0.	0000.		2665	5151
05152	ST	060100	005412	110.	0155.	ST	605.	0016.		0.	0000.		2666	5152
05153	CA	050000	205707	110.	0156.	CA	608.	0055.	B	0.	0000.	A PRIME	2667	5153
05154	FD	024000	005406	110.	0157.	FD	605.	0012.		0.	0000.	A+B	2668	5154
05155	FM	026000	206077	110.	0158.	FM	610.	0055.	B	0.	0000.	B	2669	5155
05156	FD	024000	205613	110.	0159.	FD	607.	0055.	B	0.	0000.	A	2670	5156
05157	FM	026000	205707	110.	0160.	FM	608.	0055.	B	0.	0000.	A PRIME	2671	5157
05160	FD	024000	205613	110.	0161.	FD	607.	0055.	B	0.	0000.	A	2672	5160

05161 FM	026000	001156	110.	0162.	FM	801.	0002.	0.	0000.	2	2673	5161
05162 FA	030000	005412	110.	0163.	FA	605.	0016.	0.	0000.		2674	5162
05163 FD	024000	000735	110.	0164.	FD	1.	0029.	0.	0000.	T	2675	5163
05164 FM	026000	001130	110.	0165.	FM	800.	0000.	0.	0000.	R	2676	5164
05165 FD	024000	000735	110.	0166.	FD	1.	0029.	0.	0000.	T	2677	5165
05166 SQ	-060000	005413	110.	0167.	SQ	605.	0017.	0.	0000.		2678	5166
05167 CA	050000	005413	110.	0168.	CA	605.	0017.	0.	0000.		2679	5167
05170 FS	030200	005411	110.	0169.	FS	605.	0015.	0.	0000.		2680	5170
05171 ST	060100	005414	110.	0170.	ST	605.	0018.	0.	0000.	C SUB P,ANHARM	2681	5171
05172 FA	030000	000741	110.	0171.	FA	1.	0033.	0.	0000.		2682	5172
05173 ST	060100	000741	110.	0172.	ST	1.	0033.	0.	0000.	C SUB P,TOTAL	2683	5173
05174 TX	200001	205065	110.	0178.	TX	2.	0103.	B	0.	0001.	2684	5174
05175 SDX	-053400	406226	110.	0179.	SDX	806.	0002.	C	0.	0000.	2685	5175
05176 ZS	060000	406212	110.	0180.	ZS	805.	0055.	C	0.	0000.	2686	5176
05177 TX	200001	405176	110.	0181.	TX	2.	0180.	C	0.	0001.	2687	5177
05200 SDX	-053400	106224	110.	0182.	SDX	806.	0000.	A	0.	0000.	2688	5200
05201 ZS	060000	106117	110.	0183.	ZS	804.	0011.	A	0.	0000.	2689	5201
05202 TX	200001	105201	110.	0184.	TX	2.	0183.	A	0.	0001.	2690	5202
05203 T	002000	002203	110.	0185.	T	106.	0000.		0.	0000.	2691	5203
05204 CA	050000	006227	110.	0186.	CA	806.	0003.		0.	0000.	2692	5204
05205 T	002000	005011	110.	0187.	T	2.	0062.		0.	0000.	2693	5205
05206 CA	050000	006227	110.	0188.	CA	806.	0003.		0.	0000.	2694	5206
05207 T	002000	005023	110.	0189.	T	2.	0071.		0.	0000.	2695	5207
05210 CA	050000	006227	110.	0208.	CA	806.	0003.		0.	0000.	2696	5210
05211 T	002000	005031	110.	0209.	T	2.	0075.2		0.	0000.	2697	5211
GO PRINT												
01130	201774	570651	3	800.	0000.	0.	0000.	0.	0000.	198725000000 00	600	1130
01131	202622	077325	3	800.	0001.	0.	0000.	0.	0000.	314159265350 00	601	1131
01132	114476	235455	3	800.	0002.	0.	0000.	0.	0000.	138044000000-16	602	1132
01133	052406	346323	3	800.	0003.	0.	0000.	0.	0000.	662517000000-27	603	1133
01134	243676	563112	3	800.	0004.	0.	0000.	0.	0000.	299792000000 10	604	1134
01135	317776	136520	3	800.	0005.	0.	0000.	0.	0000.	602320000000 23	605	1135
01136	224756	600400	3	800.	0006.	0.	0000.	0.	0000.	101325000000 06	606	1136
01137	205503	122254	3	800.	0007.	0.	0000.	0.	0000.	201975510000 01	607	1137
01140	203475	753412	3	800.	0008.	0.	0000.	0.	0000.	496812500000 00	608	1140
01141	205667	544466	3	800.	0009.	0.	0000.	0.	0000.	274810310000 01	609	1141
01142	202575	432477	3	800.	0010.	0.	0000.	0.	0000.	298087500000 00	610	1142
01143	201560	252000	3	800.	0011.	0.	0000.	0.	0000.	143879700000 00	611	1143

01154	000000	000000	3	801.	0000.	0.	0000.	0.	0000.	000000000000 00	620	1154
01155	201400	000000	3	801.	0001.	0.	0000.	0.	0000.	100000000000 00	621	1155
01156	202400	000000	3	801.	0002.	0.	0000.	0.	0000.	200000000000 00	622	1156
01157	203400	000000	3	801.	0003.	0.	0000.	0.	0000.	400000000000 00	623	1157
01160	175525	252521	3	801.	0004.	0.	0000.	0.	0000.	833333300000-02	624	1160
01161	171707	070677	3	801.	0005.	0.	0000.	0.	0000.	694444400000-03	625	1161
01162	202500	000000	3	801.	0006.	0.	0000.	0.	0000.	250000000000 00	626	1162
01163	201600	000000	3	801.	0007.	0.	0000.	0.	0000.	150000000000 00	627	1163
01164	173735	673605	3	801.	0008.	0.	0000.	0.	0000.	291666700000-02	628	1164
01165	177400	000000	3	801.	0009.	0.	0000.	0.	0000.	250000000000-01	629	1165
01166	173554	055374	3	801.	0010.	0.	0000.	0.	0000.	222222200000-02	630	1166
01167	177525	252514	3	801.	0011.	0.	0000.	0.	0000.	333333300000-01	631	1167
01170	175707	070673	3	801.	0012.	0.	0000.	0.	0000.	111111100000-01	632	1170
01171	174533	136455	3	801.	0013.	0.	0000.	0.	0000.	423809500000-02	633	1171
01172	200000	000000	4	801.	0014.	0.	0000.	0.	0000.	050000000000 00	634	1172
01173	211473	000000	3	801.	0015.	0.	0000.	0.	0000.	315000000000 02	635	1173
01174	175421	042107	3	801.	0016.	0.	0000.	0.	0000.	666666700000-02	636	1174
01212	201475	341217	3	802.	0000.	0.	0000.	0.	0000.	124000000000 00	650	1212
01213	205660	324773	3	802.	0001.	0.	0000.	0.	0000.	270260000000 01	651	1213
01214	201400	000000	3	802.	0002.	0.	0000.	0.	0000.	100000000000 00	652	1214
01215	201400	000000	3	802.	0003.	0.	0000.	0.	0000.	100000000000 00	653	1215
01216	000000	000000	3	802.	0004.	0.	0000.	0.	0000.	000000000000 00	654	1216
01217	201574	144435	3	802.	0005.	0.	0000.	0.	0000.	148514220000 00	655	1217
01220	000000	000000	3	802.	0006.	0.	0000.	0.	0000.	000000000000 00	656	1220
01221	214406	417270	3	802.	0007.	0.	0000.	0.	0000.	210024000000 03	657	1221
01222	201400	000000	3	802.	0008.	0.	0000.	0.	0000.	100000000000 00	658	1222
01223	212543	746314	3	802.	0009.	0.	0000.	0.	0000.	711900000000 02	659	1223
01224	202400	000000	3	802.	0010.	0.	0000.	0.	0000.	200000000000 00	660	1224
01225	214636	301727	3	802.	0011.	0.	0000.	0.	0000.	331503000000 03	661	1225
01226	201400	000000	3	802.	0012.	0.	0000.	0.	0000.	100000000000 00	662	1226
01356	206620	000000	3	803.	0000.	0.	0000.	0.	0000.	500000000000 01	750	1356
01357	206620	000000	3	803.	0001.	0.	0000.	0.	0000.	500000000000 01	751	1357
01360	211452	122250	3	803.	0002.	0.	0000.	0.	0000.	298160800000 02	752	1360
01361	211454	000000	3	803.	0003.	0.	0000.	0.	0000.	300000000000 02	753	1361
01362	207620	000000	3	803.	0004.	0.	0000.	0.	0000.	100000000000 02	754	1362
01363	212764	000000	3	803.	0005.	0.	0000.	0.	0000.	100000000000 03	755	1363
01364	215471	100000	3	803.	0006.	0.	0000.	0.	0000.	501000000000 03	756	1364
01365	212757	000000	3	803.	0007.	0.	0000.	0.	0000.	990000000000 02	757	1365
01366	210764	000000	3	803.	0008.	0.	0000.	0.	0000.	250000000000 02	758	1366
06104	155740	377564	3	804.	0000.	0.	0000.	0.	0000.	179000000000-06	3140	6104
06105	171645	312776	3	804.	0001.	0.	0000.	0.	0000.	643000000000-03	3141	6105
06106	-170472	445214	3	804.	0002.	0.	0000.	0.	0000.	-240000000000-03	3142	6106
06107	171734	747056	3	804.	0003.	0.	0000.	0.	0000.	727770000000-03	3143	6107

06123	204516	314631	3	805.	0000.	0.	0000.	0.	0000.	104500000000	01	3155	6123
06124	202563	146314	3	805.	0001.	0.	0000.	0.	0000.	290000000000	00	3156	6124
06125	204715	605075	3	805.	0002.	0.	0000.	0.	0000.	144300000000	01	3157	6125
06126	202732	702436	3	805.	0003.	0.	0000.	0.	0000.	371000000000	00	3158	6126
06127	205463	024365	3	805.	0004.	0.	0000.	0.	0000.	191900000000	01	3159	6127
06130	206644	000000	3	805.	0005.	0.	0000.	0.	0000.	525000000000	01	3160	6130

06224	000003	000000	4	806.	0000.	0.	0000.	0.	0000.	300000000000	00 17	3220	6224
06225	000062	000000	4	806.	0001.	0.	0000.	0.	0000.	500000000000	01 17	3221	6225
06226	000067	000000	4	806.	0002.	0.	0000.	0.	0000.	550000000000	01 17	3222	6226
06227	344623	713116	3	806.	0003.	0.	0000.	0.	0000.	100000000000	30	3223	6227

Appendix B
 INPUT DATA AND COMPUTED THERMODYNAMIC FUNCTIONS FOR HCN
 AS A RIGID ROTATOR-HARMONIC OSCILLATOR MOLECULE.

			HCN			
2.7025999 01	1.0000000 00	1.0000000 00	0.0000000 00	1.4851421 00	0.0000000 00	2.1002400 03
1.0000000 00	7.1189999 02	2.0000000 00	3.3150299 03	1.0000000 00	0.0000000 00	0.0000000 00
0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00
0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00
0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00
0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00
0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00
0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00
0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00
0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00
0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00
0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00

		HCN		
50.00	28.27303	6.92683	35.19986	6.95615
100.00	33.08026	6.94292	40.02318	6.97100
150.00	35.90003	6.97577	42.87580	7.15713
200.00	37.91823	7.07100	44.98923	7.58600
250.00	39.51183	7.22581	46.73764	8.10653
298.16	40.80004	7.40729	48.20733	8.58366
300.00	40.84561	7.41456	48.26017	8.60077
400.00	43.03367	7.81624	50.84991	9.40127
500.00	44.81930	8.19657	53.01587	10.01163
600.00	46.34480	8.54251	54.88730	10.52071
700.00	47.68567	8.85795	56.54362	10.97292
800.00	48.88770	9.14845	58.03615	11.38486
900.00	49.98100	9.41819	59.39919	11.76177
1000.00	50.98648	9.67000	60.65648	12.10538
1100.00	51.91931	9.90580	61.82511	12.41691
1200.00	52.79081	10.12698	62.91779	12.69806
1300.00	53.60969	10.33465	63.94434	12.95099
1400.00	54.38279	10.52979	64.91258	13.17819
1500.00	55.11559	10.71328	65.82886	13.38227
1600.00	55.81257	10.88592	66.69850	13.56575
1700.00	56.47746	11.04851	67.52596	13.73102
1800.00	57.11335	11.20175	68.31510	13.88027
1900.00	57.72291	11.34634	69.06925	14.01545
2000.00	58.30841	11.48291	69.79132	14.13828
2100.00	58.87182	11.61207	70.48388	14.25027
2200.00	59.41486	11.73435	71.14920	14.35275
2300.00	59.93905	11.85027	71.78931	14.44687
2400.00	60.44574	11.96029	72.40602	14.53361
2500.00	60.93612	12.06485	73.00096	14.61385
2600.00	61.41126	12.16433	73.57560	14.68832
2700.00	61.87214	12.25911	74.13125	14.75769
2800.00	62.31962	12.34952	74.66914	14.82252
2900.00	62.75450	12.43585	75.19035	14.88329
3000.00	63.17750	12.51840	75.69589	14.94044
3100.00	63.58927	12.59741	76.18668	14.99435
3200.00	63.99043	12.67311	76.66354	15.04533
3300.00	64.38152	12.74574	77.12726	15.09368
3400.00	64.76306	12.81548	77.57853	15.13966
3500.00	65.13552	12.88251	78.01803	15.18348
3600.00	65.49934	12.94701	78.44636	15.22535
3700.00	65.85493	13.00914	78.86407	15.26544
3800.00	66.20266	13.06902	79.27168	15.30390
3900.00	66.54288	13.12680	79.66969	15.34089
4000.00	66.87593	13.18260	80.05854	15.37651
4100.00	67.20212	13.23654	80.43865	15.41088
4200.00	67.52171	13.28870	80.81042	15.44411
4300.00	67.83500	13.33921	81.17420	15.47627
4400.00	68.14222	13.38813	81.53036	15.50745
4500.00	68.44363	13.43557	81.87919	15.53773
4600.00	68.73943	13.48159	82.22102	15.56716
4700.00	69.02985	13.52627	82.55612	15.59581
4800.00	69.31508	13.56967	82.88476	15.62373
4900.00	69.59531	13.61187	83.20719	15.65097
5000.00	69.87073	13.65292	83.52365	15.67758

Appendix C
INPUT DATA AND COMPUTED THERMODYNAMIC FUNCTIONS FOR HCN
AS A NONRIGID ROTATOR-ANHARMONIC OSCILLATOR MOLECULE

			HCN			
2.7025999 01	1.0000000 00	0.0000000 00	0.0000000 00	1.4851422 00	0.0000000 00	2.1002400 03
1.0000000 00	7.1189999 02	2.0000000 00	3.3150299 03	1.0000000 00	0.0000000 00	0.0000000 00
0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00
0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00
0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00
0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00
0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00
0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00
0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00
0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00
0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00
0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00
0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00
6.4299999-03	-2.4000000-03	7.2776999-03	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00
0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00
		1.7899999-06				
1.0449999 01	2.8999999 00	1.4429999 01	3.7099999 00	1.9189999 01	5.2499999 01	0.0000000 00
0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00
0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00
0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00
0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00
0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00
0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00
0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00
0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00	0.0000000 00

		HCN		
50.00	28.27285	6.92666	35.19950	6.95579
100.00	33.07990	6.94257	40.02247	6.97033
150.00	35.89950	6.97530	42.87481	7.15646
200.00	37.91756	7.07048	44.98805	7.58512
250.00	39.51103	7.22505	46.73608	8.10371
298.16	40.79906	7.40591	48.20497	8.57685
300.00	40.84462	7.41314	48.25777	8.59378
400.00	43.03193	7.81189	50.84382	9.38119
500.00	44.81610	8.18749	53.00360	9.97536
600.00	46.33943	8.52743	54.86687	10.46669
700.00	47.67747	8.83596	56.51344	10.89975
800.00	48.87608	9.11879	57.99486	11.29112
900.00	49.96540	9.38021	59.34561	11.64616
1000.00	50.96643	9.62312	60.58955	11.96680
1100.00	51.89435	9.84950	61.74385	12.25455
1200.00	52.76054	10.06083	62.82137	12.51134
1300.00	53.57372	10.25828	63.83200	12.73959
1400.00	54.34077	10.44289	64.78366	12.94196
1500.00	55.06721	10.61559	65.68280	13.12120
1600.00	55.75754	10.77725	66.53480	13.27995
1700.00	56.41550	10.92869	67.34420	13.42068
1800.00	57.04423	11.07068	68.11491	13.54561
1900.00	57.64640	11.20392	68.85032	13.65673
2000.00	58.22430	11.32908	69.55338	13.75579
2100.00	58.77993	11.44678	70.22671	13.84431
2200.00	59.31502	11.55760	70.87261	13.92360
2300.00	59.83110	11.66204	71.49314	13.99483
2400.00	60.32953	11.76060	72.09013	14.05896
2500.00	60.81153	11.85371	72.66524	14.11686
2600.00	61.27817	11.94178	73.21995	14.16928
2700.00	61.73044	12.02518	73.75561	14.21684
2800.00	62.16921	12.10423	74.27344	14.26010
2900.00	62.59528	12.17926	74.77454	14.29954
3000.00	63.00939	12.25055	75.25994	14.33559
3100.00	63.41219	12.31835	75.73055	14.36861
3200.00	63.80431	12.38290	76.18721	14.39891
3300.00	64.18631	12.44442	76.63072	14.42678
3400.00	64.55869	12.50311	77.06180	14.45247
3500.00	64.92194	12.55915	77.48108	14.47619
3600.00	65.27649	12.61271	77.88920	14.49813
3700.00	65.62277	12.66394	78.28672	14.51846
3800.00	65.96115	12.71300	78.67415	14.53734
3900.00	66.29199	12.76000	79.05200	14.55489
4000.00	66.61562	12.80508	79.42070	14.57123
4100.00	66.93235	12.84835	79.78069	14.58647
4200.00	67.24246	12.88990	80.13237	14.60071
4300.00	67.54624	12.92984	80.47608	14.61402
4400.00	67.84393	12.96826	80.81220	14.62650
4500.00	68.13579	13.00525	81.14103	14.63819
4600.00	68.42202	13.04086	81.46288	14.64918
4700.00	68.70285	13.07520	81.77804	14.65950
4800.00	68.97847	13.10830	82.08678	14.66922
4900.00	69.24909	13.14025	82.38934	14.67838
5000.00	69.51487	13.17110	82.68597	14.68703