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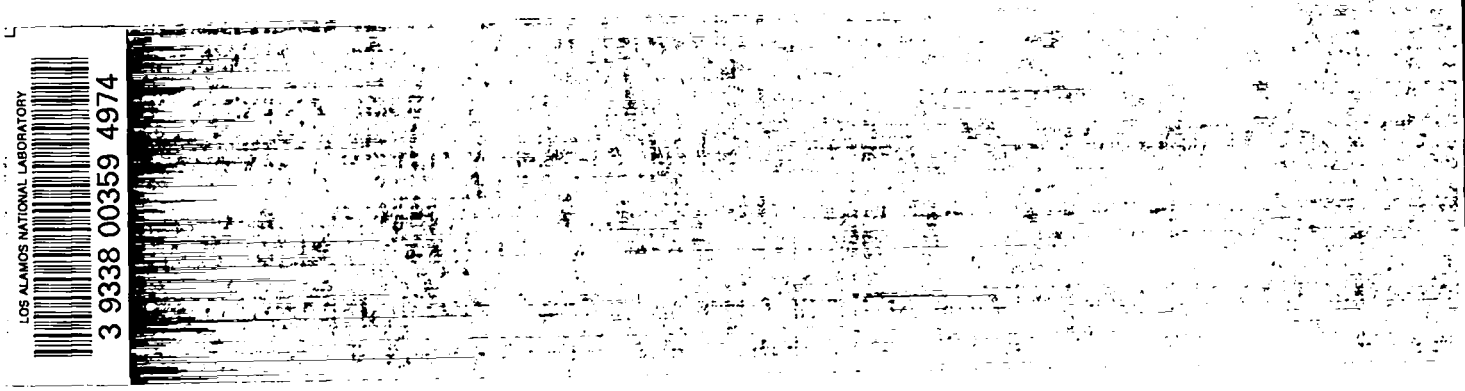
PUBCO-I, AN IBM 704 CODE FOR COMPUTING THE IDEAL THERMODYNAMIC FUNCTIONS OF A POLYATOMIC GAS MOLECULE



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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.

CONTENTS

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

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

where

g_i = degeneracy of the ith energy level,

ϵ_i = energy of the ith 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

$$Q = Q_{int} \cdot Q_{tr}. \tag{2}$$

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

$$Q = Q_{tr} \cdot Q_{el} \cdot Q_{vib} \cdot Q_{rot}. \tag{3}$$

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

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

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

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

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,

$$Q_{el} = 1. \tag{6}$$

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

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

$$Q_{vib} = \prod_i \left(\sum_{v=0}^{\infty} g_1\, e^{-hcv\omega_1/kT} \right) \left(\sum_{v=0}^{\infty} g_2\, e^{-hcv\omega_2/kT} \right) \ldots, \tag{8}$$

where

g_i = degeneracy of ith vibrational level,

c = velocity of light,

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

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

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

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

so that

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

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

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

where

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

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

Equation (11) can be expanded asymptotically to give

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

where σ is the symmetry number.

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

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

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

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

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

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

The nonrigid rotator-anharmonic oscillator molecules are treated as rigid rotator-harmonic oscillator molecules with three correction terms[3] to take care of the stretching, anharmonicity, and vibration-rotation interaction of the molecules.

The partition function for stretching is expressed as

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

where

$$\rho = 2\ kD/hcB^2. \tag{17}$$

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

The anharmonicity partition function is

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

where

g_i, g_j = vibrational degeneracies of ith and jth vibrational states,

δ_{ij} = Kronecker delta,

X_{ij} = first anharmonicity constant (cm^{-1}).

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

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

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

It is convenient to make the replacement

$$u_i = hc\nu_i/kT. \tag{20}$$

The vibration-rotation interaction partition function is expressed as

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

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

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

Enthalpy function

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

Entropy

$$S^\circ = (H^\circ - H_0^\circ)/T - (F^\circ - H_0^\circ)/T \tag{24}$$

Heat capacity

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

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:

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

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

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

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

$$\ln Q_{int} = \ln\left(Q_{vib} \cdot Q_{rot}\right) = \ln Q_{vib} + \ln Q_{rot} . \tag{29}$$

The vibrational contributions to the above thermodynamic functions are

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

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

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

The rotational contributions to the thermodynamic functions for linear molecules are

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

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

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

while for nonlinear molecules they become

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

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

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

2.3 Nonrigid Rotator-Anharmonic Oscillator Thermodynamic Functions

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

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

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

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

The anharmonicity corrections increase the thermodynamic functions by

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

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

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

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

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

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

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

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

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

$$B'' = 0. \tag{50}$$

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:

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

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

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

$$\left. - \left[\frac{g_i \delta_i \, e^{u_i} \, u_i T}{\left(e^{u_i} - 1\right)\left(e^{u_i} - 1 + g_i \delta_i\right)} \right]^2 \right\}. \tag{53}$$

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:

Card Column	Punch	Significance
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:

Column	Punch
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:

Card Columns	Punch	Significance
1	8	Control card
2-6	FWA	Initial loading address

The data cards must be punched as follows:

Card Columns	Punch	Significance
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.

Location	Operation	Address	Tag	Decrement
$(1376)_8$	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.

Location		Significance
$(1831)_{10}$	$(3447)_8$	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.

Region	Function
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

Region	Function
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:

Region	Function
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:

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

Region	Function
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}, . . . , X_{1j}, X_{22}, X_{23}, . . . , X_{2j}, X_{33}, . . . , X_{3j}, ... , 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.

2. H. S. Taylor and S. Glasstone, editors, A Treatise on Physical Chemistry, Vol. I, Atomistics and Thermodynamics., pp. 497-510, 548-572, D. Van Nostrand Company, Inc., New York, 1942.

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

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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.  MOLECULE IDENTIFICAT.   766   1376
01377 PON  100000 000362   100. 0000.2 PON   0. 0242.      0. 0000.  HALF PAGE               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.  LAS 117 PRINT FLTG      769   1401
01402 SVN -317521 101315   100. 0002.  SVN 802. 0067.  A   0. 8017.  RIGID                   770   1402
01403 SVN -317542 101316   100. 0003.  SVN 802. 0068.  A   0. 8034.  ROTATOR-               771   1403
01404 SVN -317563 101317   100. 0004.  SVN 802. 0069.  A   0. 8051.  HARMONIC               772   1404
01405 SVN -317604 101320   100. 0005.  SVN 802. 0070.  A   0. 8068.  OSCILLATOR            773   1405
01406 SVN -317625 101321   100. 0006.  SVN 802. 0071.  A   0. 8085.  DATA                   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.  SS NO. 1              779   1413
01414 T    002000 001444   100. 0012.  T     2. 0036.      0. 0000.  CALC TRANS.           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.  DELTAS               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.  STRETCH CONSTANT      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.  ANHARMONICITY         795   1433
01434 SVN -317542 106206   100. 0028.  SVN 805. 0051.  A   0. 8034.  CONSTANTS             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.  MOLECULE IDENTIFICAT.   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.  MULTIPLICITY          807   1447
01450 TSX  007400 402373   100. 0037.2 TSX 702. 0000.  C   0. 0000.  LN                    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.  R                     811   1453
01454 ST   060100 001215   100. 0037.6 ST  802. 0003.      0. 0000.  R LN MULT.            812   1454
01455 T    002000 001464   100. 0038.  T   102. 0000.      0. 0000.  CALC TRANS.          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
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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
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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
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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. 0000.  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. 0000.  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 00/707  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. 0000.  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
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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.	SQ	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.	TWO	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.	C	0.	0000.	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

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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
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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 -211704 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.   DELTAS                 1176   2230
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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.  ANHARMONICITIES       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.  READ IN NEW DATA      1181  2235
02236       000013 000000  106. 0028.        0. 0000.     0. 0011.                        1182  2236
02237       000067 000000  106. 0029.        0. 0000.     0. 0055.                        1183  2237


02241 CA    050000 002334  107. 0000.  CA  600. 0019.     0. 0000.   TEMPORARY T          1185  2241
02242 FS    030200 001366  107. 0001.  FS  803. 0008.     0. 0000.  250 DEG              1186  2242
02243 TM   -012000 002261  107. 0002.  TM    2. 0016.     0. 0000.  T LESS 250          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.  298.16              1189  2245
02246 TM   -012000 002265  107. 0005.  TM    2. 0020.     0. 0000.  T EQUAL 250         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.  T EQUAL 298         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.  INC T BY 100         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.  5010 DEG             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.  RECYCLE              1200  2260
02261 CA    050000 002334  107. 0016.  CA  600. 0019.     0. 0000.    T WKG              1201  2261
02262 FA    030000 001357  107. 0017.  FA  803. 0001.     0. 0000.  INC T BY 50          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.  RECYCLE              1204  2264
02265 CA    050000 001360  107. 0020.  CA  803. 0002.     0. 0000.  298.16              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.  RECYCLE              1207  2267
02270 CA    050000 001361  107. 0023.  CA  803. 0003.     0. 0000.  300                 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.  RECYCLE              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.  SKIP PAGE           1212  2274
02275 HP    042000 000000  107. 0027.1 HP    0. 0000.     0. 0000.  END OF PROBLEM       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.  BINARY LD           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.  STORE ZEROS         1219  2303
02304 T     002000 003472  107. 0029.  T   707. 0010.     0. 0000.  DEC LD             1220  2304
02305       000103 000000  107. 0030.        0. 0000.     0. 0067.                        1221  2305
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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. 0000.  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. 0000.                           2365  4475
04476 SDX -053400 104653  109. 0001.  SDX   2. 0105.  A   0. 0000.                           2366  4476
04477 CA   050000 201304  109. 0002.  CA  802. 0058.  B   0. 0000.  G SUB EYE               2367  4477
04500 TZ   010000 004711  109. 0003.  TZ  110. 0000.      0. 0000.  PAST LAST NU            2368  4500
04501 LQ   056000 001143  109. 0004.  LQ  800. 0011.      0. 0000.  HC/K                    2369  4501
04502 FM   026000 201303  109. 0005.  FM  802. 0057.  B   0. 0000.  NU SUB EYE             2370  4502
04503 FD   024000 000735  109. 0006.  FD    1. 0029.      0. 0000.  T                       2371  4503
04504 SQ  -060000 005245  109. 0007.  SQ  603. 0000.      0. 0000.  U SUB EYE             2372  4504
04505 CA   050000 005245  109. 0008.  CA  603. 0000.      0. 0000.                          2373  4505
04506 TSX  007400 403314  109. 0009.  TSX 704. 0000.  C   0. 0000.  EXPON                  2374  4506
04507 T    002000 004654  109. 0010.  T     2. 0106.      0. 0000.  GREATER THAN 87       2375  4507
04510 ST   060100 005246  109. 0011.  ST  603. 0001.      0. 0000.                          2376  4510
04511 FS   030200 001155  109. 0012.  FS  801. 0001.      0. 0000.  1                       2377  4511
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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

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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   A    0. 0001.                                   2471      4647
04650 TX    200002 204477    109. 0102.2  TX     2. 0002.    B    0. 0002.                                   2472      4650
04651 T     002000 004711    109. 0103.   T    110. 0000.         0. 0000.   CALC ANHARM FNS                 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
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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
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05000 ST   060100 005372   110. 0054. ST  605. 0000.      0. 0000.                    2560   5000
05001 XAD -075400 100000   110. 0055. XAD   0. 0000.  A   0. 0000.                    2561   5001
05002 CAS  034000 005372   110. 0056. CAS 605. 0000.      0. 0000.                    2562   5002
05003 T    002000 005006   110. 0057. T     2. 0060.      0. 0000.  I LESS THAN J     2563   5003
05004 T    002000 005006   110. 0058. T     2. 0060.      0. 0000.  I=J               2564   5004
05005 TX   200001 204777   110. 0059. TX    2. 0053.  B   0. 0001.  I MORE THAN J     2565   5005
05006 LQ   056000 105315   110. 0060. LQ  604. 0020.  A   0. 0000.  E TO U I - 1      2566   5006
05007 FM   026000 205315   110. 0061. FM  604. 0020.  B   0. 0000.  E TO U J - 1      2567   5007
05010 TF   014000 005204   110. 0061.1 TF    2. 0186.      0. 0000.                    2568   5010
05011 ST   060100 405613   110. 0062. ST  607. 0055.  C   0. 0000.  A SUB I,J         2569   5011
05012 LQ   056000 205341   110. 0063. LQ  604. 0040.  B   0. 0000.  NU SUB J          2570   5012
05013 FM   026000 205303   110. 0064. FM  604. 0010.  B   0. 0000.  E TO U J          2571   5013
05014 ST   060100 005375   110. 0065. ST  605. 0003.      0. 0000.                    2572   5014
05015 LQ   056000 105341   110. 0066. LQ  604. 0040.  A   0. 0000.  NU SUB I          2573   5015
05016 FM   026000 105303   110. 0067. FM  604. 0010.  A   0. 0000.  E TO U I          2574   5016
05017 ST   060100 005376   110. 0068. ST  605. 0004.      0. 0000.                    2575   5017
05020 LQ   056000 205303   110. 0069. LQ  604. 0010.  B   0. 0000.                    2576   5020
05021 FM   026000 105303   110. 0070. FM  604. 0010.  A   0. 0000.                    2577   5021
05022 TF   014000 005206   110. 0070.1 TF    2. 0188.      0. 0000.                    2578   5022
05023 ST   060100 005377   110. 0071. ST  605. 0005.      0. 0000.                    2579   5023
05024 CA   050000 205341   110. 0072. CA  604. 0040.  B   0. 0000.  NU SUB J          2580   5024
05025 FA   030000 105341   110. 0073. FA  604. 0040.  A   0. 0000.  NU SUB I          2581   5025
05026 LR   076500 000043   110. 0074. LR    0. 0035.      0. 0000.                    2582   5026
05027 FM   026000 005377   110. 0075. FM  605. 0005.      0. 0000.                    2583   5027
05030 TF   014000 005210   110. 0075.1 TF    2. 0208.      0. 0000.                    2584   5030
05031 ST   060100 005402   110. Q075.2 ST  605. 0008.      0. 0000.                    2585   5031
05032 FS   030200 005376   110. 0076. FS  605. 0004.      0. 0000.                    2586   5032
05033 FS   030200 005375   110. 0077. FS  605. 0003.      0. 0000.                    2587   5033
05034 LR   076500 000043   110. 0078. LR    0. 0035.      0. 0000.                    2588   5034
05035 FM   026000 001143   110. 0079. FM  800. 0011.      0. 0000.  HC/K              2589   5035
05036 ST   060100 405707   110. 0080. ST  608. 0055.  C   0. 0000.  A PRIME SUB I,J    2590   5036
05037 LQ   056000 005375   110. 0081. LQ  605. 0003.      0. 0000.  NU J(E TO U J)    2591   5037
05040 FM   026000 205341   110. 0082. FM  604. 0040.  B   0. 0000.  NU SUB J          2592   5040
05041 ST   060100 005400   110. 0083. ST  605. 0006.      0. 0000.                    2593   5041
05042 LQ   056000 005376   110. 0084. LQ  605. 0004.      0. 0000.  NU I(E TO U I)    2594   5042
05043 FM   026000 105341   110. 0085. FM  604. 0040.  A   0. 0000.  NU SUB I          2595   5043
05044 ST   060100 005401   110. 0086. ST  605. 0007.      0. 0000.                    2596   5044
05045 CA   050000 205341   110. 0087. CA  604. 0040.  B   0. 0000.                    2597   5045
05046 FA   030000 105341   110. 0088. FA  604. 0040.  A   0. 0000.                    2598   5046
05047 LR   076500 000043   110. 0089. LR    0. 0035.      0. 0000.                    2599   5047
05050 FM   026000 005402   110. 0090. FM  605. 0008.      0. 0000.  NU I+ NU J(E TO I+J) 2600  5050
05051 FS   030200 005400   110. 0091. FS  605. 0006.      0. 0000.                    2601   5051
05052 FS   030200 005401   110. 0092. FS  605. 0007.      0. 0000.                    2602   5052
05053 LR   076500 000043   110. 0093. LR    0. 0035.      0. 0000.                    2603   5053
05054 FM   026000 001143   110. 0094. FM  800. 0011.      0. 0000.  HC/K              2604   5054
05055 LR   076500 000043   110. 0095. LR    0. 0035.      0. 0000.                    2605   5055
05056 FM   026000 001143   110. 0096. FM  800. 0011.      0. 0000.                    2606   5056
05057 ST   060100 406003   110. 0097. ST  609. 0055.  C   0. 0000.  A DUBL PRIME I,J  2607   5057
05060 TX   200001 405061   110. 0098. TX    2. 0099.  C   0. 0001.                    2608   5060
05061 TX   200001 204777   110. 0099. TX    2. 0053.  B   0. 0001.  INCREASE J BY ONE 2609   5061
05062 SDX -053400 206224   110. 0100. SDX 806. 0000.  B   0. 0000.  RESTORE J TO 1    2610   5062
05063 TX   200001 104777   110. 0101. TX    2. 0053.  A   0. 0001.  INCREASE I BY ONE 2611   5063
05064 SDX -053400 206226   110. 0102. SDX 806. 0002.  B   0. 0000.  RESTORE B TO 55   2612   5064
05065 CA   050000 206077   110. 0103. CA  610. 0055.  B   0. 0000.  B                 2613   5065
05066 TZ   010000 002203   110. 0103.1 TZ  106. 0000.      0. 0000.  GO PRINT         2614   5066
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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.  GO PRINT                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

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.	0000000000000 00	620	1154
01155	201400 000000 3 801. 0001.	0. 0000.	0. 0000.	1000000000000 00	621	1155
01156	202400 000000 3 801. 0002.	0. 0000.	0. 0000.	2000000000000 00	622	1156
01157	203400 000000 3 801. 0003.	0. 0000.	0. 0000.	4000000000000 00	623	1157
01160	175525 252521 3 801. 0004.	0. 0000.	0. 0000.	8333333000000-02	624	1160
01161	171707 070677 3 801. 0005.	0. 0000.	0. 0000.	6944444000000-03	625	1161
01162	202500 000000 3 801. 0006.	0. 0000.	0. 0000.	2500000000000 00	626	1162
01163	201600 000000 3 801. 0007.	0. 0000.	0. 0000.	1500000000000 00	627	1163
01164	173735 673605 3 801. 0008.	0. 0000.	0. 0000.	2916667000000-02	628	1164
01165	177400 000000 3 801. 0009.	0. 0000.	0. 0000.	2500000000000-01	629	1165
01166	173554 055374 3 801. 0010.	0. 0000.	0. 0000.	2222222000000-02	630	1166
01167	177525 252514 3 801. 0011.	0. 0000.	0. 0000.	3333333000000-01	631	1167
01170	175707 070673 3 801. 0012.	0. 0000.	0. 0000.	1111111100000-01	632	1170
01171	174533 136455 3 801. 0013.	0. 0000.	0. 0000.	4238095000000-02	633	1171
01172	200000 000000 4 801. 0014.	0. 0000.	0. 0000.	0500000000000 00 00	634	1172
01173	211473 000000 3 801. 0015.	0. 0000.	0. 0000.	3150000000000 02	635	1173
01174	175421 042107 3 801. 0016.	0. 0000.	0. 0000.	6666667000000-02	636	1174
01212	201475 341217 3 802. 0000.	0. 0000.	0. 0000.	1240000000000 00	650	1212
01213	205660 324773 3 802. 0001.	0. 0000.	0. 0000.	2702600000000 01	651	1213
01214	201400 000000 3 802. 0002.	0. 0000.	0. 0000.	1000000000000 00	652	1214
01215	201400 000000 3 802. 0003.	0. 0000.	0. 0000.	1000000000000 00	653	1215
01216	000000 000000 3 802. 0004.	0. 0000.	0. 0000.	0000000000000 00	654	1216
01217	201574 144435 3 802. 0005.	0. 0000.	0. 0000.	1485142200000 00	655	1217
01220	000000 000000 3 802. 0006.	0. 0000.	0. 0000.	0000000000000 00	656	1220
01221	214406 417270 3 802. 0007.	0. 0000.	0. 0000.	2100240000000 03	657	1221
01222	201400 000000 3 802. 0008.	0. 0000.	0. 0000.	1000000000000 00	658	1222
01223	212543 746314 3 802. 0009.	0. 0000.	0. 0000.	7119000000000 02	659	1223
01224	202400 000000 3 802. 0010.	0. 0000.	0. 0000.	2000000000000 00	660	1224
01225	214636 301727 3 802. 0011.	0. 0000.	0. 0000.	3315030000000 03	661	1225
01226	201400 000000 3 802. 0012.	0. 0000.	0. 0000.	1000000000000 00	662	1226
01356	206620 000000 3 803. 0000.	0. 0000.	0. 0000.	5000000000000 01	750	1356
01357	206620 000000 3 803. 0001.	0. 0000.	0. 0000.	5000000000000 01	751	1357
01360	211452 122250 3 803. 0002.	0. 0000.	0. 0000.	2981608000000 02	752	1360
01361	211454 000000 3 803. 0003.	0. 0000.	0. 0000.	3000000000000 02	753	1361
01362	207620 000000 3 803. 0004.	0. 0000.	0. 0000.	1000000000000 02	754	1362
01363	212764 000000 3 803. 0005.	0. 0000.	0. 0000.	1000000000000 03	755	1363
01364	215471 100000 3 803. 0006.	0. 0000.	0. 0000.	5010000000000 03	756	1364
01365	212757 000000 3 803. 0007.	0. 0000.	0. 0000.	9900000000000 02	757	1365
01366	210764 000000 3 803. 0008.	0. 0000.	0. 0000.	2500000000000 02	758	1366
06104	155740 377564 3 804. 0000.	0. 0000.	0. 0000.	1790000000000-06	3140	6104
06105	171645 312776 3 804. 0001.	0. 0000.	0. 0000.	6430000000000-03	3141	6105
06106	-170472 445214 3 804. 0002.	0. 0000.	0. 0000.	-2400000000000-03	3142	6106
06107	171734 747056 3 804. 0003.	0. 0000.	0. 0000.	7277700000000-03	3143	6107

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06123  204516 314631 3 805. 0000.   0. 0000.   0. 0000.   1045000000000 01      3155  6123
06124  202563 146314 3 805. 0001.   0. 0000.   0. 0000.   2900000000000 00      3156  6124
06125  204715 605075 3 805. 0002.   0. 0000.   0. 0000.   1443000000000 01      3157  6125
06126  202732 702436 3 805. 0003.   0. 0000.   0. 0000.   3710000000000 00      3158  6126
06127  205463 024365 3 805. 0004.   0. 0000.   0. 0000.   1919000000000 01      3159  6127
06130  206644 000000 3 805. 0005.   0. 0000.   0. 0000.   5250000000000 01      3160  6130

06224  000003 000000 4 806. 0000.   0. 0000.   0. 0000.   3000000000000 00 17   3220  6224
06225  000062 000000 4 806. 0001.   0. 0000.   0. 0000.   5000000000000 01 17   3221  6225
06226  000067 000000 4 806. 0002.   0. 0000.   0. 0000.   5500000000000 01 17   3222  6226
06227  344623 713116 3 806. 0003.   0. 0000.   0. 0000.   1000000000000 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

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

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

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

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