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CALCULATION OF THE THERMODYNAMIC PROPERTIES OF GASES

L. Brewer and S. Hahn

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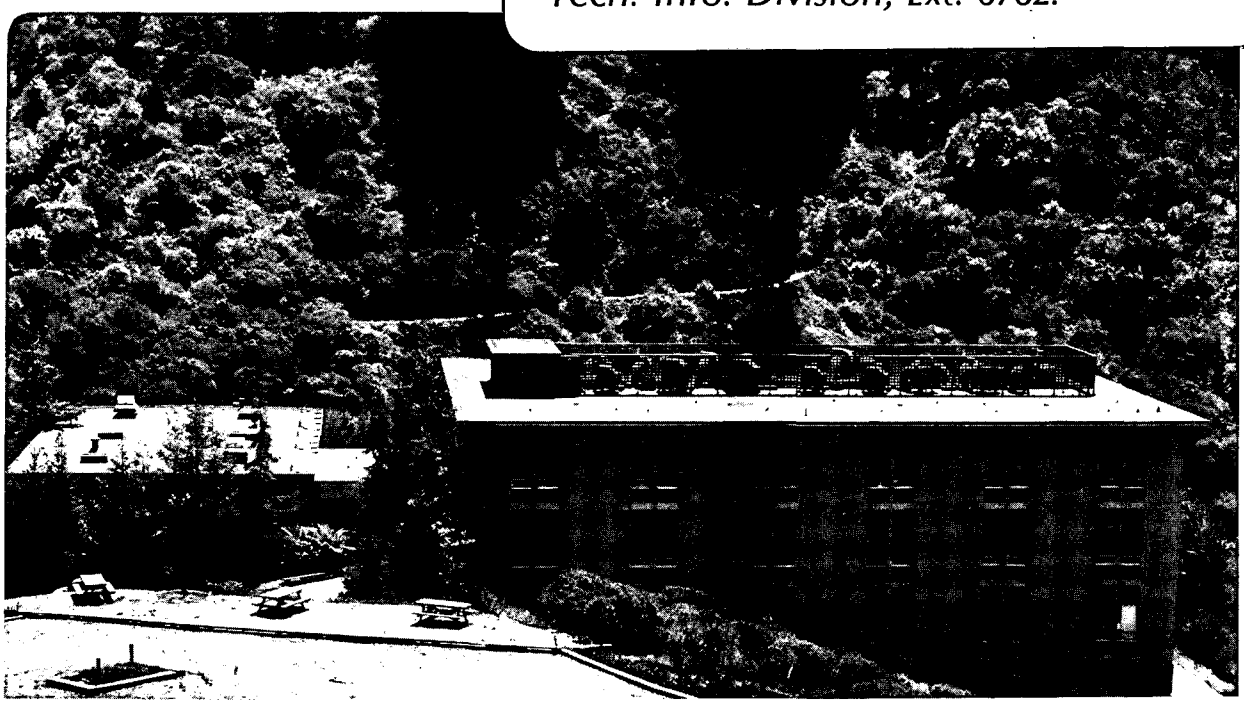

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Calculation of The Thermodynamic Properties of Gases

by

Leo Brewer and Susie Hahn

Materials and Molecular Research Division
Lawrence Berkeley Laboratory
and
Department of Chemistry
University of California
Berkeley, California 94720

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THERMODYNAMIC PROPERTIES OF GASES

The several programs tabulated here are designed to calculate the translational, electronic, vibrational and rotational contributions to the thermodynamic functions of gaseous molecules using the equations given in Chapter 27 of Ref.(1). When it is desired to obtain moments of inertia for the rotational calculations from molecular constants, Program ID can be used to calculate B_e values for diatomic or linear molecules, moments of inertia or products of inertia for a variety of molecules including bent triatomic, symmetric top CBA_3, octahedral BA_6, etc.

Program D-LT calculates the translational, rotational and vibrational contributions for diatomic or linear polyatomic molecules. For diatomic molecules, it also calculates the corrections to these results if the effects of anharmonicity, centrifugal stretching and vibration-rotation interaction are to be included. Program NL calculates the translational, rotational, and vibrational contributions for nonlinear molecules. If the values of B_e for linear molecules or the values of the products of moments of inertia for nonlinear molecules are not on hand, then Program ID must be executed before running Program D-LT or Program NL to determine these values which are used in these two programs. For gaseous atoms, Program EL provides the electronic and translational contributions to the thermodynamic functions. It can also be used to calculate only the electronic contribution for either atoms or molecules. All programs have been written for the HP41CV calculator.

The spectroscopic constants used should be expressed in units of cm^{-1}, the unit conventionally used in spectroscopic publications. All the thermodynamic quantities are calculated in dimensionless form, which is most suitable for direct calculation of equilibrium constants. However, the programs pro-

vide for multiplication by R in appropriate units to yield the functions in the units desired.

In identifying quantities, the subscripts e, r, t and v are used to refer to electronic, rotational, translational and vibrational contributions, respectively. The superscript ° for quantities including translational contributions indicates that the values are for the gaseous standard state, although the superscript is not always shown, as all values are for the gaseous standard state. Quantities to be printed are enclosed by quotation marks when it is necessary to distinguish from values only shown on calculator display.

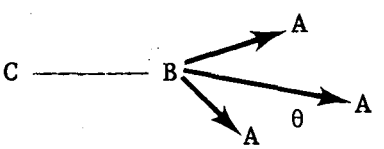
Moments of Inertia

Program ID provides the moments of inertia of molecules needed to calculate the rotational contributions to thermodynamic properties in Programs D-LT and NL. When there is more than one value, I_S is the moment about the axis of greatest symmetry. I" indicates a doubly degenerate moment. Program ID tabulates the symmetry number, σ, along with the equations for I. The number of vibrations, i_d, of degeneracy, d, are stored as $100i_1+i_2+i_3/100$ for the different types of molecules for later use in Program NL. If m is the atomic weight of A and r is the internuclear distance in Å, mr^2 must be divided by $10^{16}N_0 = 6.02209 \times 10^{39}$ to obtain units of g cm^2.

Program ID calculates $I \times 10^{39}$ in g cm^2, $B_e^* = h/8\pi^2cI$ in cm^{-1} for linear molecules, and the product of the three principal moments of inertia, $D \times 10^{117}$, for non-linear molecules. Note that Program ID does not calculate the spectroscopic value of B_e (for a single isotope) but rather the averaged-isotope value, denoted by B_e^*. (For a discussion on how to calculate thermodynamic functions from spectroscopic data, see pp. 125-26 of Ref.(1).)

For symmetric top molecules and unsymmetric linear molecules, m_1 is the atomic weight of A, m_2 of B and m_3 of C.

Molecule	σ	i_1, i_2, i_3	$100i_1+i_2+i_3/100$	Moments of Inertia
Diatomic A_2	2	1,0,0	100	$I'' = \frac{1}{2}mr^2$
Linear ABA	2	2,1,0	201	$I'' = 2mr^2$
Planar BA_3	6	2,2,0	202	$I_S = 3mr^2$
				$I'' = \frac{3}{2}mr^2$
Tetrahedral BA_4	12	1,1,2	101.02	$I = \frac{8}{3}mr^2$
Trigonal Bipyramid BA_5	6	4,4,0	404	$I_S = 3mr^2$
				$I'' = \frac{7}{2}mr^2$
Octahedral BA_6	24	1,1,4	101.04	$I = 4mr^2$
Bent BA_2	2	3,0,0	300	$I_S = mr^2\left(2 - \frac{1+\cos\theta}{1+m_B/2m}\right)$
				$I = mr^2(1+\cos\theta)/(1+2m/m_B)$
				$I = mr^2(1-\cos\theta)$

For a symmetric top 

, $\sigma = 3$, and θ in degrees

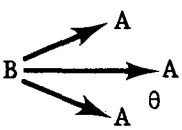
$i_1 = 3$, $i_2 = 3$, $i_3 = 0$

$100i_1 + i_2 + i_3/100 = 303$

$$I_S = 3m_1r_{12}^2(1-\cos\theta)$$

$$I'' = m_1r_{12}^2(1-\cos\theta) + \frac{m_1(m_2+m_3)r_{12}^2(1+2\cos\theta)}{3m_1+m_2+m_3}$$

$$+ \frac{m_3r_{23}}{3m_1+m_2+m_3}\left[(3m_1+m_2)r_{23} + 6m_1r_{12}\left(\frac{1+2\cos\theta}{3}\right)^{1/2}\right]$$

If $m_3 = 0$, the equations give I for the symmetric top 

, $\sigma = 3$, $i_1 = 2$, $i_2 = 2$, $i_3 = 0$, $100i_1 + i_2 + i_3/100 = 202$.

If $m_1 = 0$, I" becomes the doubly degenerate moment of inertia of diatomic CB, $\sigma = 1$.

If $\theta = 0$, I" becomes the moment of inertia of a linear triatomic molecule with atomic masses m_3, m_2 and m_1 (if m_1 is divided by three at the initiation of the program) and vibrational degeneracies $i_1 = 2$, $i_2 = 1$, and $i_3 = 0$.

Diatomic or Linear Polyatomic Gases

Program D-LT uses the rotational constants B_e^* (the averaged-isotope value, B_e^*, not the spectroscopic value, B_e), α, the symmetry number σ, the vibrational constants w_e and $x_e w_e$, and the molecular weight M. The calculations using the equations on pp. 420-30 of Ref.(1) proceed as follows with $y = hc(B_e^* - \frac{1}{2}\alpha)/kT$ and $u = hc(w_e - 2x_e w_e)/kT$.

$C_{r,t}/R = \frac{7}{2} + y^2/45$, $S_{r,t}/R = \frac{7}{2} - \ln y\sigma - y^2/90 + \frac{3}{2}\ln M - 3.665 + \frac{5}{2}\ln T$,

$-(G-H_0)_{r,t}/RT = S_{r,t}/R + y/3 + y^2/45 - \frac{7}{2}$,

$(H_{298}-H_0)_{r,t}/R = 298.15(\frac{7}{2} - \frac{1}{3}y_{298} - \frac{1}{45}y_{298}^2)$,

$-(G-H_{298})_{r,t}/RT = -(G-H_0)_{r,t}/RT + (H_{298}-H_0)_{r,t}/RT$,

$(H-H_0)_{r,t}/RT = \frac{7}{2} - \frac{1}{3}y - \frac{1}{45}y^2$,

$(H-H_{298})_{r,t}/R = [(H-H_0)_{r,t}/RT - (H_{298}-H_0)_{r,t}/RT]T$ with $-(H_{298}-H_0)_{r,t}/RT$ obtained by subtracting $-(G-H_{298})_{r,t}/RT$ from $-(G-H_0)_{r,t}/RT$ stored in the stack.

$C_v/R = u^2e^u/(e^u-1)^2$, $-(G-H_0)_v/RT = -\ln(1-e^{-u})$, $(H-H_0)_v/RT = u/(e^u-1)$,

$S_v/RT = (H-H_0)_v/RT - (G-H_0)_v/RT$, $(H_{298}-H_0)_v/R = (uT)/(e^{u_{298}} - 1)$,

$-(G-H_{298})_v/RT = -(G-H_0)_v/RT + (H_{298}-H_0)_v/RT$,

$(H-H_{298})_v/R = T[(H-H_0)_v/RT - (H_{298}-H_0)_v/RT]$.

The various contributions to $(H_{298}-H_0)/R$, C_p/R, $(H-H_{298})/R$, S/R, and $-(G-H_{298})/RT$ are summed and are stored in registers 12 to 16, respectively.

Program D-LT provides the corrections to be applied to the thermodynamic functions calculated for a diatomic molecule by the harmonic-oscillator-rigid-

rotator approximation by contributions from anharmonic centrigugal stretching, and vibration-rotation interaction. The initial spectroscopic values are used in units of cm^{-1}. The final results are first stored in registers 12 to 16 and then displayed in dimensionless form with the quantities divided by R, the gas constant. Insertion of R = 1.98719 cal/K mol or 8.3144 J $K^{-1}mol^{-1}$ will yield the values in either set of units. However, the dimensionless values are the most suitable if the values are to be used for subsequent equilibrium calculations; step 9 can be omitted if quantities in dimensions are not needed. The calculations are based on the following equations on pp. 430-7 of Ref.(1).

$$w_o = w_e - 2x_e w_e, \qquad B_o = B_e^* - \frac{1}{2}\alpha, \qquad x = w_e x_e / w_o$$

$$u = (hc/k)w_o/T = 1.4388\ w_o/T, \qquad \gamma = B_e^*/w_e, \qquad \delta = \alpha/B_o = (B_e^*/\alpha - 0.5)^{-1}$$

$$-\left(\frac{(G-H_o)}{RT}\right)_{cor} = \frac{\delta + \dfrac{2xu}{e^u-1}}{(e^u-1)} + 8\,\frac{\gamma}{u}$$

$$\left(\frac{H-H_o}{RT}\right)_{cor} = \frac{\delta u e^u + \dfrac{[2ue^u - (e^u-1)](2xu)}{(e^u-1)}}{(e^u-1)^2} + 8\,\frac{\gamma}{u}$$

$$C_{cor}/R = \frac{\delta u^2 e^u(e^u+1) + [2ue^u + u - 2(e^u-1)](2ue^u)\,\dfrac{2xu}{e^u-1}}{(e^u-1)^3} + 16\,\frac{\gamma}{u}$$

$$S_{cor} = (H-H_0)_{cor}/T - (G-H_o)_{cor}/T\ .$$

Non-Linear Gases

Program ID calculates D x 10^{117} (where D is the product of the three principal moments of inertia) and 100 $i_1 + i_2 + i_3/100$, for a variety of non-linear molecules. The following equations from Ref.(1) are used by Program NL to calculate the rotational and translational contributions to the thermo-

dynamic functions of non-linear molecules. The symmetry numbers, σ, are available in Ref.(1) and are also listed in the discussion of Program ID.

$$C^\circ_{r,t}/R = 4, \quad (H^\circ_{298}-H^\circ_0)_{r,t}/R = 4(298.15), \quad (H^\circ-H^\circ_{298})_{r,t}/R = 4(T-298.15)$$

$$S^\circ_{r,t}/R = 4 \ln T + \frac{3}{2} \ln M + \frac{1}{2}\ln(D \times 10^{117}) - \ln\sigma - 1.1823$$

$$4 + \ln 64\pi^5 + \ln(82.057k^3)/(h^6 N_0^{5/2} 10^{58.5}) = -1.1823$$

$$-(G^\circ-H^\circ_{298})_{r,t}/RT = S^\circ_{r,t}/R - 4(1 - 298.15/T).$$

The vibrational contributions are calculated using the same equations as used for Program D-LT.

The program requires that the singly degenerate vibrational frequencies be entered first followed by doubly degenerate frequencies and finally by triply degenerate frequencies. The input data is printed out in the order: first singly, then doubly, and finally triply degenerate frequencies. The number of frequencies of each type must be entered if Program ID was not previously entered. i_1 is the number of singly degenerate frequencies, i_2 is the number of doubly degenerate frequencies, and i_3 is the number of triply degenerate frequencies.

Calculation of Electronic Level Contributions to Thermodynamic Functions

Program EL can be used to calculate the complete thermodynamic functions for gaseous atoms including translational and electronic contributions or it can be used to just calculate the electronic level contributions for either atoms or molecules. Degeneracies and energies are entered and then stored for the calculations. Although the program is intended for calculating the contribution of electronic levels to thermodynamic functions, it can be used for any internal energy levels. For example, if the vibrational or rotational levels are sufficiently perturbed to introduce significant error even after

executing the correction in Program D-LT for anharmonic and centrifugal stretching corrections, the partition function can be calculated to evaluate the vibrational or rotational contributions.

The spectroscopic unit, cm^{-1}, is used for the energies. The thermodynamic functions are calculated in dimensionless units, which are most appropriate for equilibrium calculations, but insertion of the gas constant R in appropriate units will provide the thermodynamic functions in the same units. The calculations follow the equations on pp. 422-4 of Ref.(1).

After energy levels and degeneracies have been stored in the preliminary steps, calculations at various temperatures commence with step (4). There are several choices in the sequence of steps following step (4). If the interest is primarily in the complete thermodynamic functions for an atom, step (4) would be followed by step (5"a) to yield $-(G^\circ-H^\circ_{298})/RT$ and then by step (5"b) if the remainder of the functions are desired in dimensionless form. If $-(G^\circ-H^\circ_{298})/T$ is desired, step (5"a) would be followed by step (6) if the other functions are of interest. If values for all functions are wanted both with dimensions and in dimensionless form, the sequence after step (4) would be (5"a), (5"b), and (6). If only the electronic contributions are wanted, step (4) would be followed by step (5') and then by step (6) for values expressed in the units of the value of R introduced in step (6). If, after obtaining the electronic contributions of an atom through step (5'), the complete thermodynamic functions should also be wanted, replacement of the directions of step (5"a) by R↓ X<>Y R↓ M USER C will allow calculation of the complete functions without repeating step (4). The restrictions are summarized as follows: step (5"b) only after (5"a); step (6) after (5'), (5"a), or (5"b); step (5') only after (4); and step (5"a) only after (4) except after (5') with insertion of the special step given above.

REFERENCES

(1) G. N. Lewis, M. Randall, K. S. Pitzer and L. Brewer, Thermodynamics, 2nd Ed., McGraw-Hill, New York, 1961.

(2) N. Davidson, Statistical Mechanics, McGraw-Hill, New York, 1962.

PROGRAM ID

Registers

0	1	2	3	4	5	6	7	8	9
6.02209	$\frac{mr^2}{6.02209}$	$1 + \cos\Theta$	m, m_1	r_{12}	$\frac{m_1 r_{12}^2(1 - \cos\theta)}{6.02209}$	I"	m_2	m/m_B	r_{23}
	M	$\cos\Theta$	M	σ		I_s, I_1	$3m_1+m_2$	I_3	
		$1+2\cos\Theta$			$\overset{*}{Be}$ or D		I, I'', I_2	m_3	
10	11	12	13	14	15	16	17	18	19
	$100i_1+i_2+i_3/100$								

Procedure

1) 'NAME'	XEQ ID	6.022 "NAME"
2) m_1 ↑ r	USER A	$m_1 r^2/6.02209$

Print out

Diatomic A_2		r	m_1	
3D)	R/S		$\overset{*}{Be}$	M
Linear ABA		r	m_1	m_2
3LT) m_2	USER B		$\overset{*}{Be}$	M
Planar BA_3		r	m_1	m_2
3P) m_2	USER C		D	M
Tetrahedral BA_4		r	m_1	m_2
3T) m_2	USER D		D	M
Trigonal Bypyramid BA_5		r	m_1	m_2
3TB) m_2	USER E		D	M

ID, cont'd

		Print out		
Octahedral BA_6		r	m_1	m_2
30C) m_2	USER F		D	M
Bent Triatomic BA_2		r	m_1	Θ
3BT) $m_2 \uparrow \Theta$	USER H	m_2	D	M
Symmetric Top CBA_3				
2a) $r_{12} \uparrow m_1 \uparrow \Theta$	USER a	Θ	r_{12}	m_1
3a) $r_{23} \uparrow m_3 \uparrow m_2$	R/S	m_2	m_3	r_{23}
			M	D
Symmetric Top BA_3				
2b) $r_{12} \uparrow m_1 \uparrow \Theta$	USER b	Θ	r_{12}	m_1
3b) $0 \uparrow 0 \uparrow m_2$	R/S	m_2	0.000	0.000
			M	D
Linear CBA				
2c) $r_{12} \uparrow m_1$	USER c	0.000	r_{12}	$\frac{1}{3} m_1$
3c) $r_{23} \uparrow m_3 \uparrow m_2$	R/S	m_2	m_3	r_{23}
			Be*	M
Diatomic CB				
2d) $r_{23} \uparrow m_3 \uparrow m_2$	USER d	0.000	r_{12}	0.000
		m_2	m_3	r_{23}
			Be*	M

Note 1: Before executing Program ID, ensure that Flag 3 is not set.

Note 2: Steps 3D, 3LT, 3P, 3T, 3TB, 30C, and 3BT, each require Step 2 to preceed them. However, steps 2a, 2b, 2c, and 2d do not require Step 2, but rather directly follow Step 1.

PROGRAM D-LT

Registers -- Part I

0	1	2	3*	4*	5*	6	7	8	9
298.15			M	σ	B_e^*	y	yT	α	$x_e w_e$
			$\frac{3}{2}$ ln M-3.665			u			
10	11	12	13	14	15	16	17	18	19
R	$y^2/45$	$\frac{\Sigma(H_{298}-H_0)}{R}$	$\frac{\Sigma C_p}{R}$	$\frac{\Sigma(H-H_{293})}{R}$	$\frac{\Sigma S}{R}$	$\frac{\Sigma-(G-H_{298})}{RT}$	T	e^u-1	$-\ln(1-e^{-u})$
	$y/3 + y^2/45$								$\frac{(H_{298}-H_0)_v}{RT}$
	e^u								
20	21	22	23	24	25	26	27	28	29
u'T	u''T	u'''T	$\frac{u}{e^u-1}$	w_e					g index
u''T	u'T	u''T							
u'''T	u''T	u'''T							
u'T									
30	31	32	33	34	35	36	37	38	39
up to 19 values for			$\frac{-(G-H_{298})}{RT}$	→					
40	41	42	43	44	45	46	47	48	49
→									

* from Program ID

D-LT, cont'd

Registers -- Part II for Corrections to Diatomic Gas

0*	1	2	3*	4*	5*	6*	7*	8*	9*
298.15	8γ	$\frac{(H_{298}-H_0)_c}{R}$	$1.51\ln M-3.665$	σ	B_e^*	y_u	yT	α	$x_e w_e$
10*	11*	12	13	14	15	16	17	18	19*
R	$\frac{y^2}{45}$	$\frac{(H_{298}-H_0)}{R}$	$\frac{(C_p)_c}{R}$	$\frac{(H-H_{298})_c}{R}$	$\frac{S_c}{R}$	$\frac{-(G-H_{298})}{RT}$	T	u	$-\ln(1-e^{-u})$
	$y/3 + y^2/45$								$\frac{(H_{298}-H_0)_v}{RT}$
	e^u								
20*	21	22	23	24	25	26	27	28	29
uT	ue^u	e^u-1	$\frac{2xu}{(e^u-1)}$	w_e	$\frac{(H-H_0)_c}{RT}$	$\frac{-(G-H_0)_c}{RT}$	δ	x	g index
30	31	32	33	34	35	36	37	38	39
up to 19 values for $\frac{-(G-H_{298})}{RT}$ ----------→									
40	41	42	43	44	45	46	47	48	49
----------→									

* From Program D-LT Part I.

D-LT, cont'd

Procedure

If Program ID was not previously used:

0) 'NAME' GTO 'D-LT'

			Display
0a)	$\alpha \uparrow B\overset{*}{e} \uparrow \sigma \uparrow M$	USER D	1.5 ln M - 3.665
			"NAME"
2)	Proceed with Step 2		"M $B\overset{*}{e}$ α"

If Program ID was previously used, skip above and go directly to Step 1:

	Diatomic Gas		Display
1)	α	XEQ D-LT	1.5 ln M - 3.665
			"α"
2)	$w_e \uparrow x_e w_e$	R/S	uT
			"w_e $x_e w_e$"
3)	T	USER C	$-(G^\circ - H^\circ_{298})/RT$
4)		R/S	$(H^\circ_{298} - H^\circ_0)/R$
		"	S°/R
		"	C°_p/R
		"	$(H^\circ - H^\circ_{298})/R$
5)	R	R/S	$-(G^\circ - H^\circ_{298})/T$
		"	S°
		"	C°_p
		"	$(H^\circ - H^\circ_{298})$

To calculate corrections, proceed with Step 6.

6)		USER E	"$(H_{298} - H_0)_c/R$ = "
		R/S	$(S_{298})_c/R$
		"	$(C_{p298})_c/R$
7)	T	USER F	$-(G - H_{298})/RT$

D-LT, cont'd

Procedure, cont'd

8)		R/S	S_c/R
		"	C_c/R
		"	$(H-H_{298})_c/R$
9)	RCL 10	R/S	$-(G-H_{298})/T$
		"	S_c
		"	C_c
		"	$(H-H_{298})_c$
			Prints:
10)		USER G	$(H_{298}-H_0)/R$
			$-(G°-H_{298})/RT$ for each T

	Polyatomic (tri) Linear Gas		Display
1)	α	XEQ D-LT	1.5 ln M - 3.665
			"α"
2)	$w_e' \uparrow x_e w_e'$	R/S	u'T
			" w_e' $x_e w_e'$ "
2a)	$w_e'' \uparrow x_e w_e''$	USER A	u''T
			" w_e'' $x_e w_e''$ "
2b)	$w_e''' \uparrow x_e w_e'''$	USER A	u'''T
			" w_e''' $x_e w_e'''$ "
3T)	T	USER B	$-(G°-H°_{298})/RT$
4-5)	same as for diatomic gas		
			Prints:
6)		USER G	$(H_{298}-H_0)/R$
			$-(G-H_{298})/RT$ for each T

D-LT, cont'd

Note 1: For Step 0a) enter the averaged-isotope value, $\overset{*}{Be}$, not the spectroscopic value, Be.

Note 2: To calculate the thermodynamic functions for the same molecule at different temperatures, start at Step 3) or 3T) and repeat the steps which follow for each temperature. Do not, however, repeat Step 6 for the diatomic molecule.

Note 3: If α or $x_e w_e$ are not known, key zero.

Note 4: With the exception of the Gibbs Function, in Steps 6-9 only the correction term is displayed for the thermodynamic functions. In USER G, the $(H_{298}-H_0)/R$ value is printed out excluding the correction term. (This value can be added to the $(H_{298}-H_0)_c/R$ value obtained in USER E to yield the total value for this function). However, the correction term is included in the print out of $-(G-H_{298})/RT$.

PROGRAM NL

Registers

0	1	2	3	4	5	6	7	8	9
298.15	$S_{r,t}/R$ $-4 \ln T$		M	σ	D	u	e^u $\frac{u}{e^u - 1}$	e^u-1	$-\ln(1-e^{-u})$ $\frac{(H_{298}-H_0)_v}{RT}$
10	11*	12	13	14	15	16	17	18	19
R	$100i+i_2+i_3/100$	$\frac{\Sigma(H_{298}-H_0)}{R}$	$\frac{\Sigma C_p}{R}$	$\frac{\Sigma(H-H_{298})}{RT}$	$\frac{\Sigma S}{R}$	$\frac{\Sigma -(G-H_{298})}{RT}$	T		
20	21	22	23	24	25	26	27	28	29
									g index
	$i_1/1000$	$i_2/1000$	$i_3/1000$						

NL, cont'd

Registers, cont'd

30	31	32	33	34	35	36	37	38	39
up to 19 values of $\frac{-(G-H_{298})}{RT}$ ----------→									
40	41	42	43	44	45	46	47	48	49 vibration index
50	51	52	53	54	55	56	57	58	59
values of uT ----------→									

* From Program ID

Procedure

If Program ID was not previously used:

0) 'NAME' GTO 'NL'

			Display
0a)	D x 10^{117} ↑ σ ↑ M	USER E	0.000 "NAME" "M D"

Proceed with Step 2)

If Program ID was previously used, skip above and go directly to step 1):

1)		XEQ NL	0.000

For step 2), enter the types of degeneracies in separate groups, not more than three at a time. For example:

2)	w_3' ↑ w_2' ↑ w_1'	USER A	"w_1' w_2' w_3' "
	w_4'	" 1st singly degenerate	" w_4' "
	w_2'' ↑ w_1''	" then doubly	" w_1'' w_2'' "
	w_1'''	" then triply	" w_1''' "

NL, cont'd

Procedure, cont'd

3)		USER B	0.000
	or if Program ID was not executed:		
	3') $i_1 \uparrow i_2 \uparrow i_3$	USER b	0.000 "i_1" "i_2" "i_3"
4)	T	USER C	$-(G^\circ-H^\circ_{298})/RT$
5)		R/S	$(H^\circ_{298}-H^\circ_0/R$
		"	S°/R
		"	C°_p/R
		"	$(H-H^\circ_{298})/R$
6)	R	R/S	$-(G^\circ-H^\circ_{298})/T$
		"	S°
		"	C°_p
		"	$(H-H^\circ_{298})$
			Prints:
7)		USER D	$(H^\circ_{298}-H^\circ_0/R$ $-(G^\circ - H_{298})/RT$ for each T

Note 1: If Program ID was executed previously, Step 3') which calculates $100i_1+i_2+i_3/100$ is not required because Program ID already calculated this value and stored it in R11.

Note 2: Calculations at each temperature start at Step 4.

PROGRAM EL

Registers

0	1	2	3	4	5	6	7	8	9
298.15	1438.8	3.665							$\frac{-(G-H_0)}{RT}$
10	11	12	13	14	15	16	17	18	19
R		$\frac{\Sigma(H_{298}-H_0)}{R}$	Q"	$\frac{\Sigma(H-H_{298})}{R}$	Q'	Q $\frac{-(G-H_{298})}{RT}$	T		Index
			C_p/R		Q'/Q S/R				
20	21	22	23	24	25	26	27	28	29 g index
30	31	32	33	34	35	36	37	38	39
up to 19 values of $\frac{-(G-H_{298})}{RT}$ ----------→									
40	41	42	43	44	45	46	47	48	49 Electronic Index
----------→									
50	51	52	53	54	55	56	57	58	59
values for 1438.8 $\varepsilon_i \cdot g_i \times 10^{-2}$ ----------→									

Procedure

1-1) $g_1 \uparrow \varepsilon_1$	XEQ EL	1438.8 $\varepsilon_1 \cdot g_1 \times 10^{-2}$
		" g_1 ε_1 "
1-2) $g_2 \uparrow \varepsilon_2$	R/S	1438.8 $\varepsilon_2 \cdot g_2 \times 10^{-2}$
		" g_2 ε_2 "
1-i) $g_i \uparrow \varepsilon_i$	"	1438.8 $\varepsilon_i \cdot g_i \times 10^{-2}$
		" g_i ε_i "
2)	USER A	$(H_{298}-H_0)_e/R$

EL, cont'd

Procedure cont'd

3)		R/S	$(S_{298}/R)_e$
		"	$(C_{298}/R)_e$
4)*	T	USER B	"$-(G-H_{298})_e/RT$ = "
5')	(not to be followed by 5"a without step given in text)	R/S	$(H-H_{298})_e/R$
		"	S_e/R
		"	C_e/R
5"a)	M	USER C	$(H-H_{298})/R$
5"b)		R/S	$-(G°-H°_{298})/RT$
		"	$S°/R$
		"	$C°_p/R$
6)	R	USER D	$(H-H_{298})$
		R/S	$-(G°-H°_{298})/T$
		"	$S°$
		"	$C°_p$
			Prints:
7)		USER E	$(H_{298}-H_0)_e/R$
			$-(G°-H_{298})/RT$
			for each T

* Flow Path:
1), 2), 3), 4), 5'), 6), 7) or 1), 2), 3), 4), 5"a), 5"b), 6), 7)
Also see text.

Note 1: If a number of levels are inserted together at an average value of ε_i, the total g must not exceed 99.

Note 2: If values of ε_i larger than 69 502 cm^{-1} are to be used, change constant in register 01 to 143.88 and change 1000 at step 72 to 100 to allow values up to 695 000 cm^{-1}. With this change, ε values are truncated beyond .01 cm^{-1}.

Note 3: The dimensionless values for functions at 298 K given by Steps 2 and 3 can be multiplied by R by the following procedure. After Step 3, key R in the desired units followed by USER D to display $(H-H_{298})_e$. Then R/S will displa the electronic contributions $-(G-H_{298})_e/T$, S_e, and C_e.

Note 4: If $-(G-H_0)/RT$ is desired, it can be obtained after step 4 or any of the following steps by keying RCL 09. Keying of e^x would then give Q, the partition function.

Note 5: Registers 12 to 16 first contain electronic terms only and then total terms.

TEST CALCULATIONS (Printer Attached in MAN Mode)

Diatomic A_2

ID	1)	'CU_2'	XEQ'ID'	6.022
				"CU_2"
	2)	m = 63.546 ↑ r = 2.2197	USER A	51.991
	3D)		R/S	"2.220 63.546
				0.108 127.092"
D-LT	1)	$\alpha = 6.14 \times 10^{-4}$	XEQ'D-LT'	3.602
		OR		"0.001"
		0) 'CU_2'	GTO 'D-LT'	
		0a) $\alpha = 6.14 \times 10^{-4}$ ↑ B_e* = 0.1076845 ↑ σ = 2 ↑ M = 127.092		
			USER D	3.602
				"CU_2"
				"127.092 0.108 0.001"
	2)	ω_e = 264.55 ↑ $x_e\omega_e$ = 1.025	R/S	377.685
				"264.550 1.025"
	3)	T = 3000	USER C	35.331
	4)		R/S	1,191,624
			"	39.372
			"	4.499
			"	12,123.444
	5)	R = 1.98719	R/S	70.209
			"	78.240
			"	8.940

Diatomic A_2, cont'd

6)		USER E	"$(H_{298} - H_0)_c/R$ = 3.093"
		R/S	0.017
		"	0.025
7)	T = 3000	USER F	35.455
8)		R/S	0.256
		"	0.267
		"	395.513
9)	RCL 10	R/S	70.456
		"	0.509
		"	0.530
		"	785.960
10)		USER G	"$(H_{298} - H_0)/R$ = 1,191.624"
			"35.455"

Linear ABA

ID	1)	'LI$_2$O'	XEQ 'ID'	6.022
				"LI$_2$O"
	2)	m = 6.941 ↑ r = 1.60	USER A	2.951
	3LT)	m_B = 15.9994	USER B	1.600 6.941 15.999
				0.474 29.881
D-LT	1)	α = 0	XEQ'D-LT'	1.431
		OR		"0.000"
		0) 'LI$_2$O'	GTO 'D-LT'	
		0a) α = 0 ↑ B_e^* = 0.47436 ↑ σ = 2 ↑ M = 29.8814		
			USER D	1.431
				"LI$_2$O"
				"29.881 0.474 0.000"
	2)	ω_e' = 760 ↑ $x_e\omega_e'$ = 0	R/S	1093.488
				"760.000 0.000"
	2a)	ω_e'' = 140 ↑ $x_e\omega_e''$ = 0	USER A	201.432
				"140.000 0.000"
	2b)	ω_e''' = 987 ↑ $x_e\omega_e'''$ = 0	USER A	1,420.096
				"987.000 0.000"
	3T)	T = 3000	USER B	35.448
	4)		R/S	1,305.108
			"	41.872
			"	7.452

Linear ABA cont'd

5)	R = 1.98719	R/S	70.442
		"	83.208
		"	14.808
		"	38,299.109
6)		USER G	"$(H_{298} - H_0)/R$ = 1,305.108"
			"35.448"

Diatomic CB

ID	1)	'LaO'	XEQ 'ID'	6.022
				"LaO"
	2d)	$r_{23} = 1.8257 \uparrow m_3 = 138.9055 \uparrow m_2 = 15.9994$		
			USER d	"0.000 1.826 0.000
				15.999 138.906 1.826
				0.353 154.905"
D-LT	1)	$\alpha = 0.0014$	XEQ 'D-LT'	3.899
		OR		"0.001"
		0) 'LaO'	GTO 'D-LT'	
		0a) $\alpha = 0.0014 \uparrow B_e^* = 0.35252 \uparrow \sigma = 1 \uparrow M = 154.9049$		
			USER D	3.899
				"LaO"
				"154.905 0.353 0.001"
	2)	$\omega_e = 812.75 \uparrow x_e\omega_e = 2.222$	R/S	1162.99
				"812.750 2.222"
	3)	T = 3000	USER C	34.093
	4)		R/S	1067.367
			"	38.056
			"	4.488
			"	11,888.446
	5)	R = 1.98719	R/S	67.750
			"	75.625
			"	8.918
			"	23,624.601

Diatomic CB cont'd

6)		USER E	"$(H_{298} - H_0)_c/R = 0.382$"
		R/S	0.002
7)	T = 3000	USER F	34.120
8)		R/S	0.059
		"	0.067
		"	97.164
9)	RCL 10	R/S	67.804
		"	0.118
		"	0.132
		"	193.083
10)		USER G	"$(H_{298} - H_0)/R = 1067.367$"
			"34.120"

Linear CBA

ID	1)	'COS'	XEQ 'ID'	6.022
				"COS"
	2c)	$r_{12} = 1.16 \uparrow m_1 = 15.9994$	USER c	"0.000 1.160 5.333"
	3c)	$r_{23} = 1.56 \uparrow m_3 = 32.06 \uparrow m_2 = 12.011$		
			R/S	"12.011 32.060 1.56
				0.203 60.070"
D-LT	1)	$\alpha = 0.0$	XEQ 'D-LT'	2.478
		OR		"0.000"
		0) "COS"	GTO 'D-LT'	
		0a) $\alpha = 0 \uparrow B_e^* = 0.2029 \uparrow \sigma = 1 \uparrow M = 60.070$		
			USER D	2.478
				"COS"
				"60.070 0.203 0.000"
	2)	$\omega_e' = 859 \uparrow x_e\omega_e' = 2$	R/S	1230.174
				"859.000 2.000"
	2a)	$\omega_e'' = 2064 \uparrow x_e\omega_e'' = 3.5$	USER A	2959.612
				"2064.000 3.500"
	2b)	$\omega_e''' = 524 \uparrow x_e\omega_e''' = 0.2$	USER A	753.356
				"524.000 0.200"
	3T)	$T = 3000$	USER B	36.696
	4)		R/S	1194.632
			"	42.952
			"	7.398
			"	18769.895

Linear CBA cont'd

5)	R = 1.98719	R/S	72.921
		"	85.354
		"	14.702
		"	37299.348
6)		USER G	"$(H_{298} - H_0)/R$ = 1194.632"
			"36.696"

Planar BA_3

ID	1)	'OSO_3'	XEQ 'ID'	6.022
				"OSO_3"
	2)	m_1 = 15.9994 ↑ r = 1.85	USER A	9.093
	3P	m_2 = 190.2	USER C	"1.850 15.999 190.200 5074.620 238.198"
NL	1)		XEQ 'NL'	0.000
		OR		
		0) 'OSO_3'	GTO 'NL'	
		0a) D x 10^{117} = 5074.620 ↑ σ = 6 ↑ M = 238.198		
			USER E	0.000
				"OSO_3"
				"238.198 5074.620"
	2)	ω_1' = 764 ↑ ω_2' = 291	USER A	0.000
				"291.000 764.000"
		ω_1'' = 811 ↑ ω_2'' = 292	USER A	0.000
				"292.000 811.000"
	3)		USER B	0.000
		OR if Program ID was not previously executed:		
		3') i_1 = 2 ↑ i_2 = 2 ↑ i_3 = 0	USER b	"2.000"
				"2.000"
				"0.000"
	4)	T = 3000	USER C	44.420
	5)		R/S	1516.741
			"	51.424
			"	7.973
			"	21011.780

6)	R = 1.98719	R/S	88.271
		"	102.189
		"	15.844
		"	41754.399
7)		USER D	"$(H_{298} - H_0)/R$ = 1516.741"
			"44.420"

Tetrahedral BA_4

ID	1)	'OSO_4'	XEQ 'ID'	6.022
				"OSO_4"
	2)	m_1 = 15.9994 ↑ r = 1.85	USER A	9.093
	3T)	m_2 = 190.2	USER D	"1.850 15.999 190.200 14256.271 254.198"
NL	1)		XEQ 'NL'	0.000
		OR		
		0) 'OSO4'	GTO 'NL'	
		0a) D x 10^{117} = 14256.271 ↑ σ = 12 ↑ M = 254.198		
			USER E	0.000
				"OSO_4"
				"254.198 14256.271"
	2)	ω_1' = 971	USER A	0.000
				"971.000"
		ω_1'' = 328	USER A	0.000
				"328.000"
		ω_1''' = 959.7 ↑ ω_2''' = 328	USER A	0.000
				"328.000 959.700"
	3)		USER B	0.000
		OR if Program ID was not previously executed:		
		3') i_1 = 1 ↑ i_2 = 1 ↑ i_3 = 2	USER b	"1.000"
				"1.000"
				"2.000"
	4T)	T = 3000	USER C	43.775

Tetrahedral BA_4 cont'd

5)		R/S	1463.158
		"	50.707
		"	7.961
		"	20795.137
6)	R = 1.98719	R/S	86.990
		"	100.764
		"	15.819
		"	41323.888
7)		USER D	"$(H_{298} - H_0)/R$ =
			"1463.158"
			"43.775"

Trigonal Bypyramid BA_5

ID	1)	'MOCL$_5$'	XEQ 'ID'	6.022
				"MOCL$_5$"
	2)	m_1 = 35.453 ↑ r = 2.27	USER A	30.336
	3TB)	m_2 = 95.94	USER E	"2.270 35.453 95.940
				1025958.356 273.205"
NL	1)		XEQ 'NL'	0.000
		OR		
		0) 'MOCL$_5$'	GTO 'NL'	
		0a) D x 10^{117} = 1025958.356 ↑ σ = 6 ↑ M = 273.205		
			USER E	0.000
				"MOCL$_5$"
				"273.205 1025958.356"
	2)	ω_1' = 490 ↑ ω_2' = 400 ↑ ω_3' = 410	USER A	0.000
				"410.000 400.000 490.000"
		ω_4' = 150	USER A	0.000
				"150.000"
		ω_1'' = 350 ↑ ω_2'' = 170 ↑ ω_3'' = 100	USER A	0.000
				"100.000 170.000 350.000"
		ω_4'' = 190	USER A	0.000
				"190.000"

Trigonal Bypyramid BA_5 cont'd

3)		USER B	0.000
	OR if Program ID was not previously executed:		
	3') $i_1 = 4 \uparrow i_2 = 4 \uparrow i_3 = 0$	USER B	4
			4
			0
4)	T = 3000	USER C	58.797
5)		R/S	2381.729
		"	69.477
		"	11.985
		"	32037.723
6)	R = 1.98719	R/S	116.842
		"	138.063
		"	23.816
		"	63665.043
7)		USER D	"$(H_{298} - H_0)/R$ = 2381.729"
			"58.797"

Octahedral BA_6

ID	1)	'$MOCL_6$'	XEQ 'ID'	6.022
				"$MOCL_6$"
	2)	$m_1 = 35.453 \uparrow r = 2.27$	USER A	30.336
	30C)	$m_2 = 95.94$	USER F	"2.270 35.453 95.940
				1786702.987 308.658"
NL	1)		XEQ 'NL'	0.000
		OR		
		0) '$MOCL_6$	GTO 'NL'	
		0a) $D \times 10^{117} = 1786702.987 \uparrow \sigma = 24 \uparrow M = 308.658$		
			USER E	0.000
				"$MOCL_6$"
				"308.658 1786702.987"
	2)	$\omega_1' = 347$	USER A	0.000
				"347.000"
		$\omega_1'' = 326$	USER A	0.000
				"326.000"
		$\omega_1''' = 390 \uparrow \omega_2''' = 144 \uparrow \omega_3''' = 171$		
			USER A	0.000
				"171.000 144.000 390.000"
		$\omega_4''' = 106$	USER A	0.000
				"106.000"

Octahedral BA_6 cont'd

3)		USER B	0.000
	OR if Program ID was not previously executed:		
	3') $i_1 = 1 \uparrow i_2 = 1 \uparrow i_3 = 4$	User b	1
			1
			4
4)	T = 3000	USER C	54.010
5)		R/S	2157.943
		"	62.944
		"	9.992
		"	26799.758
6)	R = 1.98719	R/S	107.329
		"	125.081
		"	19.855
		"	53256.211
7)		USER D	"$(H_{298} - H_0)/R$ = 2157.943"
			"54.010

Symmetric Top CBA_3

ID	1)	'CF_3I'	XEQ 'ID'	6.022
				"CF_3I"
	2a)	$r_{12} = 1.332 \uparrow m_1 = 18.9984 \uparrow \theta = 108.3$		
			USER a	"108.300 1.332 18.998"
	3a)	$r_{23} = 2.134 \uparrow m_3 = 126.9045 \uparrow m_2 = 12.011$		
			R/S	"12.011 126.905 2.134 195.911 44346.193"
NL	1)		XEQ 'NL'	0.000
	OR			
	0)	'CF_3I'	GTO 'NL'	
	0a)	$D \times 10^{117} = 44346.193 \uparrow \sigma = 3 \uparrow M = 195.911$		
			USER E	0.000
				"CF_3I"
				"195.911 44346.193"
	2)	$\omega_1' = 1073 \uparrow \omega_2' = 741 \uparrow \omega_3' = 286$	USER A	0.000
				"286.000 741.000 1073.000"
		$\omega_1' = 1185 \uparrow \omega_2'' = 540 \uparrow \omega_3'' = 265$	USER A	0.000
				"265.000 540.000 1185.000"
	3)		USER B	0.000
	OR if Program ID was not previously executed:			
	3')	$i_1 = 3 \uparrow i_2 = 3 \uparrow i_3 = 0$	USER b	"3"
				"3"
				"0"
	4)	T = 3000	USER C	48.150

Symmetric Top CBA_3 cont'd

5)		R/S	1584.983
		"	56.709
		"	9.933
		"	25675.901
6)	R = 1.98719	R/S	95.684
		"	112.692
		"	19.738
		"	51022.893
7)		USER D	"$(H_{298} - H_0)/R$ = 1584.983"
			"48.150"

Symmetric Top BA_3

ID	1)	'MOO$_3$ TOP'	XEQ 'ID'	6.022
				"MOO$_3$ TOP"
	2b)	r_{12} = 1.73 ↑ m_1 = 15.9994 ↑ θ = 99	User b	"99.000 1.730 15.999"
	3b)	0 ↑ 0 ↑ m_2 = 95.94	R/S	"95.940 0.000 0.000"
				"143.938 3030.655"
				143.9382
NL	1)		XEQ 'NL'	0.000
		OR		
		0) 'MOO$_3$ TOP'	GTO 'NL'	
		0a) D x 10^{117} = 3030.655 ↑ σ = 3 ↑ M = 143.938		
			USER E	0.000
				"MOO$_3$ TOP"
				"143.938 3030.655"
	2)	ω_1' = 978 ↑ ω_2' = 340	USER A	0.000
				"340.000 978.000"
		ω_1'' = 924 ↑ ω_2'' = 310	USER A	0.000
				"310.000 924.000"
	3)		USER B	0.000
		OR if Program ID was not previously executed:		
		3') i_1 = 2 ↑ i_2 = 2 ↑ i_3 = 0	User b	"2"
				"2"
				"0"
	4)	T = 3000	USER C	43.579

Symmetric Top BA_3 cont'd

5)		R/S	1467.221
		"	50.517
		"	7.962
		"	20812.775
6)	R = 1.98719	R/S	86.600
		"	100.386
		"	15.821
		"	41358.939
7)		USER D	"$(H_{298} - H_0)/R$ = 1467.221"
			"43.579"

Bent BA_2

ID	1)	'Bent CS_2O'	XEQ 'ID'	6.022
				"Bent CS_2O"
	2)	m_1 = 132.9054 ↑ r = 2.28	USER A	114.727
	3BT)	m_2 = 15.9994 ↑ θ = 140	USER H	"2.280 132.905 140.000
				15.999 63027.920 281.810"
NL	1)		XEQ 'NL'	0.000
	OR			
		0) 'Bent CS_2O'	GTO 'NL'	
		0a) D x 10^{117} = 63027.92 ↑ σ = 2 ↑ M = 281.81		
			USER E	"Bent CS_2O"
				"281.810 63027.920"
	2)	ω_3' = 455 ↑ ω_2' = 60 ↑ ω_1' = 305	USER A	0.000
				"305.000 60.000 455.000"
	3)		USER B	0.000
	OR if Program ID was not			
	previously executed:			
		3') i_1 = 3 ↑ i_2 = 0 ↑ i_3 = 0	USER b	"3.000"
				"0.000"
				"0.000"
	4)	T = 3000	USER C	47.878
	5)		R/S	1662.346
			"	54.133
			"	6.994
			"	18765.196

Bent BA_2 cont'd

6)	R = 1.98719	R/S	95.143
		"	107.573
		"	13.899
		"	37290.009
7)		USER D	"$(H_{298} - H_0)/R$ = 1662.346"
			"47.878"

Electronic Contribution for $MoCl_5$

'$MOCL_5$'	PRINT	"$MOCL_5$"			
1-1) $g_1 = 2 \uparrow \varepsilon_1 = 0$	XEQ 'EL'	0.020			
		"2.000 0.000"			
1-2) $g_2 = 2 \uparrow \varepsilon_2 = 1000$	R/S	1,433,800.020			
		"2.000 1000.000"			
1-3) $g_3 = 2 \uparrow \varepsilon_3 = 7500$	"	10,791,000.02			
		"2.000 7500.000"			
2)	USER A	11.448			
3)	R/S	0.740			
	"	0.184			
4) T = 3000	USER B	"$-(G-H_{298})_e/RT$ = 1.196"			
5"a) M = 273.205	USER C	7463.762	5')	R/S	709.137
5"b)	R/S	26.210		"	1.432
	"	28.698		"	0.244
	"	2.744			
6) R = 1.98719	USER D	14,831.913	6) R = 1.98719	USER D	1409.190
	R/S	52.085		R/S	2.376
	"	57.029		"	2.846
	"	5.453		"	0.485
7)	USER E	"$(H_{298} - H_0)_e/R$ = 11.448"		USER E	"$(H_{298} - H_0)_e/R$ = 11.448"
		"26.210"			"26.210"

OR

Flow path
1), 2), 3), 4), 5"a), 5"b), 6), 7)
or 1), 2), 3), 4), 5'), 6), 7)

```
 01♦LBL "ID"
6.02209  STO 00  FIX 3
PRA  RTN

 07♦LBL A
ACX  X↑2  X<>Y  STO 03
ACX  *  RCL 00  /
STO 01  RTN  2  STO 04
ST* 03  1/X  PRBUF
XEQ 00  GTO 01

 25♦LBL B
ACX  PRBUF  2  STO 04
ST* 03  RDN  ST+ 03  2
XEQ 00

 35♦LBL 01
STO 07  2.79932  X<>Y  /
STO 05  ACX  RCL 03  ACX
ADV  RTN

 46♦LBL C
202  STO 11  RDN  ACX
ADV  3  XEQ 04  6
STO 04  3  XEQ 00
STO 06  1.5  XEQ 00
GTO 02

 62♦LBL D
101.02  STO 11  RDN  ACX
PRBUF  4  XEQ 04  12
STO 04  8  ENTER↑  3  /
XEQ 00  ENTER↑  GTO 02


 79♦LBL E
404  STO 11  RDN  ACX
PRBUF  5  XEQ 04  6
STO 04  3  XEQ 00
STO 06  3.5  XEQ 00
GTO 02

 95♦LBL F
101.04  STO 11  RDN  ACX
PRBUF  6  XEQ 04  24
STO 04  4  XEQ 00
ENTER↑

108♦LBL 02
STO 07  X↑2  *  ACX
STO 05  RCL 03  ACX  ADV
RTN

118♦LBL 00
RCL 01  *  RTN

122♦LBL 04
ST* 03  RDN  ST+ 03  RTN


127♦LBL H
300  STO 11  RDN  ACX
PRBUF  COS  1  +  STO 02
X<>Y  ACX  RCL 03  2
STO 04  ST* 03  RDN
X<>Y  ST+ 03  /  STO 08
1/X  2  +  /  1  -  CHS
2  *  XEQ 00  STO 06
RCL 02  RCL 08  2  *  1
+  /  XEQ 00  STO 07  2
RCL 02  -  XEQ 00
STO 08  *  *  STO 05
ACX  RCL 03  ACX  ADV
RTN

181♦LBL a
303  STO 11  RDN

185♦LBL 05
ACX  COS  STO 02  RDN
X<>Y  STO 04  XEQ A
PRBUF  1  RCL 02  -
RCL 01  *  STO 05  2  *
RCL 02  2  *  1  +
STO 02  X<>Y  STO 06
RTN
```

```
211♦LBL 03
STO 07  ACX  X<>Y
STO 08  ACX  +  RCL 01
*  X<>Y  STO 09  ACX
ADV  RDN  RCL 03  3  *
RCL 07  +  STO 07
RCL 08  +  STO 01  /
RCL 02  *  RCL 05  +
RCL 02  3  /  SQRT
RCL 03  *  6  *  RCL 04
*  RCL 07  RCL 09  *  +
RCL 08  *  RCL 01
STO 03  FC? 03  ACX  /
RCL 00  /  RCL 09  *  +
STO 07  X↑2  RCL 06  *
STO 05  FC? 03  ACX
FC? 03  ADV  3  STO 04
RTN

277♦LBL b
202  STO 11  RDN  GTO 05

282♦LBL c
SF 03  3  /  0  XEQ 05
RTN  GTO 06

290♦LBL d
SF 03  STO 07  CLX  RDN
STO 08  CLX  RDN  STO 09
RDN  RDN  XEQ 05  RCL 09
RCL 08  RCL 07

305♦LBL 06
XEQ 03  3  ST/ 04
RCL 07  XEQ 01  CF 03
RTN  .END.
```

313 steps
459 bytes
69 registers

```
 01♦LBL "D-LT"
STO 08  ACX  FIX 3
PRBUF  2  /  CHS  RCL 05
+  1.4388  STO 01  *
STO 07  RCL 03  LN  1.5
*  3.665  -  STO 03
30.1  STO 29  RDN  STOP

 26♦LBL 00
X<>Y  STO 24  ACX  X<>Y
STO 09  ACX  ADV  XEQ 01
STO 20  RTN

 37♦LBL 01
2  *  -  1.4388  *  RTN

 44♦LBL D
PRA  STO 03  ACX  RDN
STO 04  RDN  STO 05  ACX
RDN  GTO "D-LT"

 55♦LBL A
X<>Y  ACX  X<>Y  ACX
ADV  XEQ 01  FS? 03
GTO 02  STO 21  SF 03
RTN

 67♦LBL 02
STO 22  RTN

 70♦LBL B
SF 03  XEQ C  RCL 21
XEQ 03  STO 21  XEQ 04
RCL 22  XEQ 03  STO 22
XEQ 04  XEQ 04  RCL 21
XEQ 03  RCL 22  STO 21
RDN  STO 22  CF 03
GTO 05

 90♦LBL 03
RCL 20  X<>Y  STO 20
RDN  RTN
```

```
 96♦LBL C
0  STO 13  STO 15  RDN
STO 17  RCL 07  X<>Y  /
STO 06  X↑2  45  /
STO 11  3.5  +  ST+ 13
RCL 04  RCL 06  *  LN
CHS  3.5  +  RCL 11  2
/  -  RCL 03  +  RCL 17
LN  2.5  *  +  ST+ 15
RCL 06  3  /  RCL 11  +
STO 11  +  3.5  -
RCL 07  3  /  298.15
STO 00  /  ENTER↑  X↑2
5  /  +  3.5  -  RCL 00
*  CHS  STO 12  RCL 17
/  +  STO 16  -  RCL 11
-  3.5  +  RCL 17  *
STO 14

170♦LBL 04
RCL 20  RCL 17  /
STO 06  X↑2  LASTX  E↑X
STO 11  *  LASTX  1  -
STO 18  X↑2  /  ST+ 13
RCL 11  RCL 18  /  LN
STO 19  RCL 06  RCL 18
/  STO 23  +  ST+ 15
RCL 19  RCL 06  RCL 20
RCL 00  /  E↑X  1  -  /
STO 19  +  ST+ 16  -
RCL 23  +  RCL 17  *
ST+ 14  RCL 19  RCL 17
*  ST+ 12  FS? 03  RTN


222♦LBL 05
RCL 16  STO IND 29  STOP
RCL 12  STOP  RCL 15
STOP  RCL 13  STOP
RCL 14  RTN  STO 10
RCL 16  *  STOP  RCL 10
RCL 15  *  STOP  RCL 10
RCL 13  *  STOP  RCL 10
RCL 14  *  RTN
```

```
250♦LBL E
RCL 09  RCL 24  RCL 09
2  *  -  /  STO 28
RCL 05  8  *  RCL 24  /
STO 01  RCL 05  RCL 08
/  .5  -  1/X  STO 27
RCL 00  SF 04  XEQ F
CF 04  RCL 25  RCL 17  *
STO 02  "<H298-H0>c/R="
PRA  PRX  RTN  RCL 15
STOP  RCL 13  RTN

288♦LBL F
STO 17  RCL 20  X<>Y  /
STO 18  ENTER↑  E↑X  1
-  STO 22  /  2  *
RCL 28  *  STO 23
RCL 27  +  RCL 22  /
RCL 01  RCL 18  /  +
STO 26  RCL 18  ENTER↑
E↑X  *  STO 21  2  *
RCL 22  -  RCL 23  *
RCL 21  RCL 27  *  +
RCL 22  X↑2  /  RCL 01
RCL 18  /  +  STO 25
RCL 21  2  *  RCL 18  +
RCL 22  2  *  -  RCL 21
*  2  *  RCL 23  *
RCL 27  RCL 22  2  +  *
RCL 21  *  RCL 18  *  +
RCL 22  3  Y↑X  /
RCL 01  2  *  RCL 18  /
+  STO 13  RCL 25
RCL 17  *  FS? 04
RCL 12  FC? 04  RCL 02
-  STO 14  RDN  RCL 26
RCL 25  +  STO 15
FS? 04  RCL 12  FC? 04
RCL 02  RCL 17  /
RCL 26  +  FS? 04  RTN
ST+ 16  RCL 16
STO IND 29  ISG 29  STOP
RCL 15  STOP  RCL 13
STOP  RCL 14  RTN
RCL 16  *  STOP  RCL 10
RCL 15  *  STOP  RCL 10
RCL 13  *  STOP  RCL 10
RCL 14  *  RTN
```

```
423♦LBL G
"(H298-H0)/R="  PRA
RCL 12  PRX  RCL 29  1.1
-  1000  /  30  +
PRREGX  RTN  .END.
```

437 steps
668 bytes
96 registers

```
 01♦LBL "NL"
0  RCL 05  SQRT  RCL 04
/  LN  RCL 03  LN  1.5
*  +  1.1823  -  STO 01
CLX  50.049  STO 49
30.1  STO 29  CLX  RTN

 23♦LBL A
ACX  1.4388  *
STO IND 49  ISG 49  CLX
R↑  CLX  RDN  RDN  X=0?
GTO 06  GTO A

 37♦LBL E
PRA  STO 03  ACX  RDN
STO 04  RDN  STO 05  ACX
PRBUF  GTO "NL"

 48♦LBL B
RCL 11  FRC  STO 23
LASTX  INT  1 E2  /
ENTER↑  FRC  STO 22  RDN
INT  1 E3  /  STO 21  10
ST/ 22  ST/ 23  CLX  RTN

 69♦LBL b
STO 23  RDN  STO 22  RDN
STO 21  21.023  PRREGX
1 E3  ST/ 23  ST/ 22
ST/ 21  CLX  RTN

 83♦LBL C
STO 17  LN  4  *  RCL 01
+  STO 15  4  STO 13
RCL 17  *  298.15
STO 00  4  *  STO 12  -
STO 14  RCL 17  /  -
STO 16  RCL 21  STO 49
X≠0?  XEQ 02  RCL 22
ST+ 49  X≠0?  XEQ 03
RCL 23  ST+ 49  X≠0?
XEQ 03  GTO 05
```

```
119♦LBL 02
50.049  ST+ 49

122♦LBL 03
XEQ 04  ISG 49  GTO 03
RTN

127♦LBL 04
RCL IND 49  RCL 17  /
STO 06  X↑2  LASTX  E↑X
STO 07  *  LASTX  1  -
STO 08  X↑2  /  ST+ 13
RCL 07  RCL 08  /  LN
STO 09  RCL 06  RCL 08
/  STO 07  +  ST+ 15
RCL 09  RCL 06
RCL IND 49  RCL 00  /
E↑X  1  -  /  STO 09  +
ST+ 16  -  RCL 07  +
RCL 17  *  ST+ 14
RCL 09  RCL 17  *
ST+ 12  RTN

178♦LBL 05
RCL 16  STO IND 29
ISG 29  STOP  RCL 12
STOP  RCL 15  STOP
RCL 13  STOP  RCL 14
RTN  STO 10  RCL 16  *
STOP  RCL 10  RCL 15  *
STOP  RCL 10  RCL 13  *
STOP  RCL 10  RCL 14  *
RTN

207♦LBL 06
ADV  RTN

210♦LBL D
"(H298-H0)/R="  PRA
FIX 3  RCL 12  PRX
RCL 29  1.1  -  1000  /
30  +  PRREGX  RTN  END
```

225 steps
366 bytes
53 registers

```
 01♦LBL "EL"
50.3  STO 49  30.1
STO 29  RDN  RDN

 08♦LBL 00
X<>Y  ACX  X<>Y  ACX
PRBUF  1438.8  STO 01  *
INT  X<>Y  100  /  +
STO IND 49  ISG 49  RTN
GTO 00

 26♦LBL A
XEQ 01  0  STO 12
298.15  STO 00  STO 17
XEQ 02  SF 04  XEQ 03
CF 04  R↑  STO 12
STO 14  RTN  RCL 15
STOP  RCL 13  RTN

 45♦LBL B
STO 17  XEQ 01  XEQ 02
GTO 03

 50♦LBL 01
0  STO 13  STO 15
STO 16  RCL 49  1.3  -
1000  /  50  +  STO 19
RTN

 64♦LBL 02
RCL IND 19  ENTER↑  FRC
100  *  X=0?  RTN  X<>Y
INT  1000  /  RCL 17  /
ENTER↑  RDN  CHS  E↑X  *
ST+ 16  R↑  *  ST+ 15
LASTX  *  ST+ 13  ISG 19
GTO 02  RTN
```

```
 93♦LBL 03
RCL 13  RCL 16  /
RCL 15  RCL 16  /
STO 15  X↑2  -  STO 13
RCL 15  RCL 17  *
RCL 12  -  RCL 16  LN
STO 09  RCL 15  +
STO 15  RCL 12  RCL 17
/  RCL 09  +  STO 16
FS? 04  RTN
"-(G-H298)e/RT="  PRA
PRX  RTN  R↑  STO 14
STOP  RCL 15  STOP
RCL 13  RTN

134♦LBL C
R↑  X<>Y  LN  LASTX
RCL 17  *  LN  2.5
ST+ 13  *  X<>Y  -
3.665  STO 02  -  ENTER↑
ENTER↑  RCL 09  +
STO 09  RDN  ENTER↑
ENTER↑  2.5  +  ST+ 15
RDN  RCL 00  RCL 17  /
2.5  *  +  ST+ 16  RDN
RCL 17  RCL 00  -  2.5
*  +  STO 14

177♦LBL 04
RTN  RCL 16  STO IND 29
ISG 29  STOP  RCL 15
STOP  RCL 13  RTN

187♦LBL D
STO 10  RCL 14  *  STOP
RCL 10  RCL 16  *  STOP
RCL 10  RCL 15  *  STOP
RCL 10  RCL 13  *  RTN


204♦LBL E
"(H298-H0)/R="  PRA
FIX 3  RCL 12  PRX
RCL 29  1.1  -  1000  /
30  +  PRREGX  RTN
.END.
```

219 steps
360 bytes
52 registers

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TECHNICAL INFORMATION DEPARTMENT
LAWRENCE BERKELEY LABORATORY
UNIVERSITY OF CALIFORNIA
BERKELEY, CALIFORNIA 94720