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PROPERTIES OF GASES

L. Brewer and S. Hahn

December 1983

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Calculation of The
Thermodynamic Properties of Gases

by

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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 , $B_e^* = h/8\pi^2 cI$ 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	$I_S = mr^2(2 - \frac{1+\cos\theta}{1+m_B/2m})$ $I = mr^2(1+\cos\theta)/(1+2m/m_B)$ $I = mr^2(1-\cos\theta)$

$\sigma = 3$, 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 $u = hc(w_e - 2x_e w_e)/kT$.

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

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

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

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

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

$$(H-H_{298})_{r,t}/R = [(H-H_0)_{r,t}/RT - (H_{298}-H_0)_{r,t}/RT]T \text{ with } -(H_{298}-H_0)_{r,t}/RT$$

obtained by subtracting $-(G-H_{298})_{r,t}/RT$ from $-(G-H_0)_{r,t}/RT$ stored in the stack.

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

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

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

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

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 centrifugal 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 $R = 1.98719 \text{ cal/K mol}$ or $8.3144 \text{ J K}^{-1}\text{mol}^{-1}$ 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).

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

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

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

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

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

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

Non-Linear Gases

Program ID calculates $D \times 10^{117}$ (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.

$$C_{r,t}^{\circ}/R = 4, (H_{298}^{\circ} - H_0^{\circ})_{r,t}/R = 4(298.15), (H^{\circ} - H_{298}^{\circ})_{r,t}/R = 4(T - 298.15)$$

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

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

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

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 $-(G^\circ - H_{298}^\circ)/RT$ and then by step (5"b) if the remainder of the functions are desired in dimensionless form. If $-(G^\circ - H_{298}^\circ)/T$ 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

<u>Registers</u>									
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	
		$1+2\cos\theta$			$Be^* \text{ or } D$		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) $m_1 \uparrow r$

USER A

 $m_1 r^2 / 6.02209$ Print outDiatomic A₂

3D)

R/S

r	m_1	
	Be^*	M

Linear ABA3LT) m_2

USER B

r	m_1	m_2
	Be^*	M

Planar BA₃3P) m_2

USER C

r	m_1	m_2
	D	M

Tetrahedral BA₄3T) m_2

USER D

r	m_1	m_2
	D	M

Trigonal Bypyramid BA₅3TB) m_2

USER E

r	m_1	m_2
	D	M

ID, cont'dPrint outOctahedral BA₆30C) m_2

USER F

r	m_1	m_2
	D	M

Bent Triatomic BA₂3BT) $m_2 \uparrow \theta$

USER H

r	m_1	θ
m_2	D	M

Symmetric Top CBA₃2a) $r_{12} \uparrow m_1 \uparrow \theta$

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 BA₃2b) $r_{12} \uparrow m_1 \uparrow \theta$

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 CBA2c) $r_{12} \uparrow m_1$

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 CB2d) $r_{23} \uparrow m_3 \uparrow m_2$

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, 3OC, and 3BT, each require Step 2 to precede 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	Be^*	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	$y^2/45$	$\frac{\Sigma(H_{298} - H_0)}{R}$	$\frac{\Sigma C_p}{R}$	$\frac{\Sigma(H - H_{298})}{R}$	$\frac{\Sigma S}{R}$	$\frac{\Sigma - (G - H_{298})}{RT}$	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	$8\gamma \frac{(H_{298}-H_0)_c}{R}$		$1.51nM-3.665$	σ	Be^*	y_u	yT	α	$x_e w_e$
10*	11*	12	13	14	15	16	17	18	19*
R	$\frac{y^2}{45}$	$\frac{(H_{298}-H_0)_c}{R}$	$\frac{(C_p)_c}{R}$	$\frac{(H-H_{298})_c}{R}$	$\frac{S_c}{R}$	$\frac{-(G-H_{298})_c}{RT}$	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}	$\frac{2 \times u}{(e^u-1)}$	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			$\frac{-(G-H_{298})_c}{RT}$						
40	41	42	43	44	45	46	47	48	49

* From Program D-LT Part I.

D-LT, cont 'dProcedure

If Program ID was not previously used:

0) 'NAME' GTO 'D-LT'

Display

0a)	$\alpha \uparrow Be^* \uparrow \sigma \uparrow M$	USER D	$1.5 \ln M - 3.665$
			"NAME"
2)	Proceed with Step 2		"M Be [*] α "

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

Diatomic GasDisplay

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	$-(G^\circ - H_{298}^\circ)/RT$
4)		R/S	$(H_{298}^\circ - H_0^\circ)/R$
		"	S°/R
		"	C_p°/R
		"	$(H^\circ - H_{298}^\circ)/R$
5)	R	R/S	$-(G^\circ - H_{298}^\circ)/T$
		"	S°
		"	C_p°
		"	$(H^\circ - H_{298}^\circ)$

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'dProcedure, 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	$(H_{298} - H_0)/R$
			$-(G^\circ - H_{298})/RT$
			for each T

Polyatomic (tri) Linear GasDisplay

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	$-(G^\circ - H_{298}^\circ)/RT$
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, B_e^* , not the spectroscopic value, B_e .

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	$e^u - 1$	$-\ln(1 - e^{-u})$
							$\frac{u}{e^u - 1}$		$\frac{(H_{298} - H_0)_v}{RT}$
10	11*	12	13	14	15	16	17	18	19
R	$100i_1 + i_2 + i_3/100$	$\frac{\Sigma(H_{298} - H_0)}{R}$	$\frac{\Sigma C_p}{R}$	$\frac{\Sigma(H - H_{298})}{RT}$	$\frac{\Sigma S}{R}$	$\frac{\Sigma -(G - H_{298})}{RT}$	T		
20	21	22	23	24	25	26	27	28	29
	$i_1/1000$	$i_2/1000$	$i_3/1000$						g index

NL, cont'dRegisters, 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'

0a) $D \times 10^{117} \uparrow \sigma \uparrow M$

USER E

Display

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) $w_3' \uparrow w_2' \uparrow w_1'$ USER A"w₁' w₂' w₃' " w_4' " 1st singly degenerate" w₄' " $w_2'' \uparrow w_1''$ " then doubly" w₁'' w₂'' " w_1''' " then triply" w₁''' "

NL, cont'dProcedure, 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	$-(G^\circ - H_{298}^\circ)/RT$
5)		R/S	$(H_{298}^\circ - H_0^\circ)/R$
		"	S°/R
		"	C_p°/R
		"	$(H - H_{298}^\circ)/R$
6)	R	R/S	$-(G^\circ - H_{298}^\circ)/T$
		"	S°
		"	C_p°
		"	$(H - H_{298}^\circ)$
			<u>Prints:</u>
7)		USER D	$(H_{298}^\circ - H_0^\circ)/R$
			$-(G^\circ - H_{298}^\circ)/RT$
			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.

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	$-(G^\circ-H_{298}^\circ)/RT$
		"	S°/R
		"	C_p°/R
6)	R	USER D	$(H-H_{298})$
		R/S	$-(G^\circ-H_{298}^\circ)/T$
		"	S°
		"	C_p°
<u>Prints:</u>			
7)		USER E	$(H_{298}-H_0)_e/R$
			$-(G^\circ-H_{298}^\circ)/RT$
			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 $69\,502\text{ cm}^{-1}$ 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 $695\,000\text{ cm}^{-1}$. With this change, ϵ values are truncated beyond $.01\text{ cm}^{-1}$.
- 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 display 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
			"0.001"
		OR	
		0) 'CU ₂ '	GTO 'D-LT'
		0a) $\alpha = 6.14 \times 10^{-4} \uparrow B_e^* = 0.1076845 \uparrow \sigma = 2 \uparrow M = 127.092$	
			USER D 3.602
			"CU ₂ "
			"127.092 0.108 0.001"
	2)	$\omega_e = 264.55 \uparrow x_e \omega_e = 1.025$	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 A₂, 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 ω _e ' = 0	R/S	1093.488
			"760.000 0.000"	
	2a)	ω _e '' = 140 ↑ x _e ω _e '' = 0	USER A	201.432
			"140.000 0.000"	
	2b)	ω _e ''' = 987 ↑ x _e ω _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)	'La0'	XEQ 'ID'	6.022
				"La0"
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
				"0.001"
		OR		
		0) 'La0'	GTO 'D-LT'	
		0a) $\alpha = 0.0014 \uparrow B_e^* = 0.35252 \uparrow \sigma = 1 \uparrow M = 154.9049$		
			USER D	3.899
				"La0"
				"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 BA₃

ID	1)	'OSO ₃ '	XEQ 'ID'	6.022
				"OSO ₃ "
	2)	$m_1 = 15.9994 \uparrow r = 1.85$	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)	GTO 'NL'	
		0a)		
		$D \times 10^{117} = 5074.620 \uparrow \sigma = 6 \uparrow M = 238.198$		
			USER E	0.000
				"OSO ₃ "
				"238.198 5074.620"
	2)	$\omega_1' = 764 \uparrow \omega_2' = 291$	USER A	0.000
				"291.000 764.000"
		$\omega_1'' = 811 \uparrow \omega_2'' = 292$	USER A	0.000
				"292.000 811.000"
	3)		USER B	0.000
		OR if Program ID was not previously executed:		
		3')		
		$i_1 = 2 \uparrow i_2 = 2 \uparrow i_3 = 0$	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 BA₄

ID	1)	'OSO ₄ '	XEQ 'ID'	6.022
				"OSO ₄ "
	2)	$m_1 = 15.9994 \uparrow r = 1.85$	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)	'OS04'	GTO 'NL'
		0a)	$D \times 10^{117} = 14256.271 \uparrow \sigma = 12 \uparrow M = 254.198$	
			USER E	0.000
				"OSO ₄ "
				"254.198 14256.271"
	2)	$\omega_1' = 971$	USER A	0.000
				"971.000"
		$\omega_1'' = 328$	USER A	0.000
				"328.000"
		$\omega_1''' = 959.7 \uparrow \omega_2''' = 328$	USER A	0.000
				"328.000 959.700"
	3)		USER B	0.000
		OR if Program ID was not		
		previously executed:		
		3')	$i_1 = 1 \uparrow i_2 = 1 \uparrow i_3 = 2$	USER b
				"1.000"
				"1.000"
				"2.000"
	4T)	$T = 3000$	USER C	43.775

Tetrahedral BA₄ 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 BA₅

ID	1)	'MOCL ₅ '	XEQ 'ID'	6.022
				"MOCL ₅ "
	2)	$m_1 = 35.453 \uparrow r = 2.27$	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)	$D \times 10^{117} = 1025958.356 \uparrow \sigma = 6 \uparrow M = 273.205$	
			USER E	0.000
				"MOCL ₅ "
				"273.205 1025958.356"
	2)	$\omega_1' = 490 \uparrow \omega_2' = 400 \uparrow \omega_3' = 410$	USER A	0.000
				"410.000 400.000 490.000"
		$\omega_4' = 150$	USER A	0.000
				"150.000"
		$\omega_1'' = 350 \uparrow \omega_2'' = 170 \uparrow \omega_3'' = 100$	USER A	0.000
				"100.000 170.000 350.000"
		$\omega_4'' = 190$	USER A	0.000
				"190.000"

Trigonal Bypyramid BA₅ cont'd

3)	OR if Program ID was not previously executed:	USER B	0.000
	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 BA₆

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 BA₆ cont'd

3)	OR if Program ID was not previously executed:	USER B	0.000
	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 CBA₃

ID	1)	'CF ₃ I'	XEQ 'ID'	6.022
				"CF ₃ I"
	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 ₃ I'	GTO 'NL'
		0a)	$D \times 10^{117} = 44346.193 \uparrow \sigma = 3 \uparrow M = 195.911$	
			USER E	0.000
				"CF ₃ I"
				"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 CBA₃ 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 BA₃

ID	1)	'MOO ₃ TOP'	XEQ 'ID'	6.022
				"MOO ₃ TOP"
	2b)	$r_{12} = 1.73 \uparrow m_1 = 15.9994 \uparrow e = 99$	User b	"99.000 1.730 15.999"
	3b)	$0 \uparrow 0 \uparrow m_2 = 95.94$	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)	$D \times 10^{117} = 3030.655 \uparrow \sigma = 3 \uparrow M = 143.938$	
			USER E	0.000
				"MOO ₃ TOP"
				"143.938 3030.655"
	2)	$\omega_1' = 978 \uparrow \omega_2' = 340$	USER A	0.000
				"340.000 978.000"
		$\omega_1'' = 924 \uparrow \omega_2'' = 310$	USER A	0.000
				"310.000 924.000"
	3)		USER B	0.000
		OR if Program ID was not previously executed:		
		3')	$i_1 = 2 \uparrow i_2 = 2 \uparrow i_3 = 0$	User b
				"2"
				"2"
				"0"
	4)	$T = 3000$	USER C	43.579

Symmetric Top BA₃ 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"

<u>Bent BA₂</u>		
ID	1) 'Bent CS ₂ O'	XEQ 'ID' 6.022 "Bent CS ₂ O"
	2) $m_1 = 132.9054 \uparrow r = 2.28$	USER A 114.727
	3BT) $m_2 = 15.9994 \uparrow \theta = 140$	USER H "2.280 132.905 140.000 15.999 63027.920 281.810"
NL	1)	XEQ 'NL' 0.000
	OR 0) 'Bent CS ₂ O'	GTO 'NL'
	0a) $D \times 10^{117} = 63027.92 \uparrow \sigma = 2 \uparrow M = 281.81$	USER E "Bent CS ₂ O" "281.810 63027.920"
	2) $\omega_3' = 455 \uparrow \omega_2' = 60 \uparrow \omega_1' = 305$	USER A 0.000 "305.000 60.000 455.000"
	3)	USER B 0.000
	OR if Program ID was not previously executed:	
	3') $i_1 = 3 \uparrow i_2 = 0 \uparrow i_3 = 0$	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 BA₂ 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 MoCl₅

'MOCL ₅ '	PRINT	"MOCL ₅ "
1-1) $g_1 = 2 \uparrow \epsilon_1 = 0$	XEQ 'EL'	0.020
		"2.000 0.000"
1-2) $g_2 = 2 \uparrow \epsilon_2 = 1000$	R/S	1,433,800.020
		"2.000 1000.000"
1-3) $g_3 = 2 \uparrow \epsilon_3 = 7500$	"	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"

OR

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 =	USER E	"(H ₂₉₈ - H ₀) _e /R =	
		11.448"			11.448"
		"26.210"			"26.210"

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 X12 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 X12 * 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 08 / RCL 09 * +
STO 07 X12 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
RT 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"

```

```

49*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 X12 LASTX E1X
STO 07 * LASTX 1 -
STO 08 X12 / 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 /
E1X 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

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 R1 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 ENTER1 FRC
100 * X=0? RTN X<>Y
INT 1000 / RCL 17 /
ENTER1 RDN CHS E1X *
ST+ 16 R1 * ST+ 15
LASTX * ST+ 13 ISG 19
GTO 02 RTN

225 steps
366 bytes
53 registers

```

93*LBL 03
RCL 13 RCL 16 /
RCL 15 RCL 16 /
STO 15 X12 - 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 R1 STO 14
STOP RCL 15 STOP
RCL 13 RTN

```

```

134*LBL C
R1 X<>Y LN LASTX
RCL 17 * LN 2.5
ST+ 13 * X<>Y -
3.665 STO 02 - ENTER1
ENTER1 RCL 09 +
STO 09 RDN ENTER1
ENTER1 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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