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MASTER

STRETCH TDF

A CODE FOR COMPUTING THERMODYNAMIC FUNCTIONS

by

William R. Gage

Charles L. Mader

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LOS ALAMOS SCIENTIFIC LABORATORY

of the

UNIVERSITY OF CALIFORNIA

GMX-2-R-64-2

STRETCH TDF

A CODE FOR COMPUTING THERMODYNAMIC FUNCTIONS

by

William R. Gage
Charles L. Mader

Report written:
August, 1964

STRETCH TDF - A CODE FOR COMPUTING THERMODYNAMIC FUNCTIONS

By William R. Gage and Charles L. Mader

ABSTRACT

This report is a description of a code for the IBM 7030 computer for computing the ideal gas thermodynamic function for monoatomic, diatomic, and polyatomic gases and the thermodynamic functions for solids. The output of the calculations is designed to be the input to the STRETCH BKW code.

STRETCH TDF is a translation and integration of the GMX-2 thermodynamic function codes for the 7094³. For monoatomic, diatomic, and polyatomic gases STRETCH TDF will calculate the free energy, the enthalpy, and the entropy as a function of temperature. These functions are then fit to a 4th degree polynomial by the method of least squares. The integration constant IC in the equation $H^{\circ} - H_{\circ}^{\circ} = \int T \frac{\partial S}{\partial T} dT + IC$ is computed from the fit of entropy as a function of temperature. As an option, the moments of inertia can be found in the polyatomic case. For one Debye Theta and two Debye Theta solids, the heat capacity is computed as a function of temperature in addition to the above quantities. The output from STRETCH TDF is designed for input to STRETCH BKW^{1,2} and is similar to that found in previous GMX-2 reports³.

A detailed description of the equations may be found in the appendix.

INPUT

The following is a list of units for input parameters.

Molecular weight grams/mole
Temperature °K
Moments of inertia gm-cm² x 10³⁹
Fundamental frequency 1/cm
Vibrational frequency 1/cm
Anharmonic coefficient 1/cm
Rotational coefficient 1/cm
Rotational-Vibrational coefficient ... 1/cm
Term value of electronic state 1/cm
Coordinates for moment of inertia Å
Debye Theta °K

INPUT FORMAT FOR STRETCH TDF

1st card - Identification (col 2-80) (Format H+ +)

2nd card - Col 2-5 type of molecule as follows: (Format V1*4)

0001	monoatomic gas
0002	diatomic gas
0003	polyatomic gas
0004	1 theta solid
0005	2 theta solid

INPUT FOR MONOATOMIC GAS

3rd card - (Format EO.1.11.3)
col 1-18 Molecular weight (grams/mole)

4th card (Format 3EO.1.11.3)
col 1-18 Initial temperature (°K)
col 19-36 Temperature increment (°K)
col 37-54 Final temperature (°K)
Note: Maximum number of temperatures is 1000.

5th card - (Format EO.1.11.3, V1*4)
col 1-18 Go E Statistical weight of 0th state
col 20-23 N2 - The number of electronic states
(may be 0, maximum of 30)
Note: This is the last card if N2 = 0.

6th and following cards - (Format 2EO.1.11.3)
col 1-18 Term value of ith electronic state (1/cm)
col 19-36 Statistical weight of ith electronic state

INPUT FOR DIATOMIC GAS

- 3rd card - (Format 2E0.1.11.3)
col 1-18 Molecular weight (grams/mole)
col 19-36 Symmetry number
- 4th card - (Format 3E0.1.11.3)
col 1-18 Initial temperature (°K)
col 19-36 Temperature increment (°K)
col 37-54 Final temperature (°K)
Note: No more than 1000 temperatures may be specified.
- 5th card - (Format 4E0.1.11.3)
col 1-18 We - Vibrational frequency (1/cm)
col 19-36 WeXe - Anharmonic coefficient (1/cm)
col 37-54 Be - Rotational coefficient (1/cm)
col 55-72 Ae - Rotational-Vibrational coefficient (1/cm)
- 6th card - (Format E0.1.11.3, V1*4)
col 1-18 Go E Statistical weight of 0th state
col 20-23 N2 - The number of electronic states
(may be 0, maximum of 30)
Note: This is the last card if N2 = 0.
- 7th and following cards - (Format 2E0.1.11.3)
col 1-18 Term value of ith electronic state (1/cm)
col 19-36 Statistical weight of ith electronic state

INPUT FOR POLYATOMIC GAS

3rd card - (Format 2E0.1.11.3)
col 1-18 Molecular weight (grams/mole)
col 19-36 Symmetry number

4th card - (Format 3E0.1.11.3)
col 1-18 Initial temperature (°K)
col 19-36 Temperature increment (°K)
col 37-54 Final temperature (°K)
Note: No more than 1000 temperatures may be specified.

5th card - (Format 3V1*4)
col 2-5 L, L = 0 for linear molecule, L = 1 for non-linear molecule
col 7-10 NA, NA = 0 if moments of inertia are read in. Otherwise, NA is number of atoms in a molecule for the moment of inertia calculation.
col 12-15 NUM, Number of fundamental frequencies (may be 0, maximum of 10)

For NA = 0

6th card - (Format 3E0.1.11.3)
col 1-18, 19-36, 37-54 Moments of inertia ($\text{gm-cm}^2 \times 10^{39}$)
(If the molecule is linear, only the 1st moment, col 1-18, need be entered.)

7th card - (Format E0.1.11.3)
col 1-18 Go E Statistical weight of the 0th state
Note: This is the last card if NUM = 0.

8th and following card - (Format 2E0.1.11.3)
col 1-18 Fundamental frequency (1/cm)
col 19-36 Degeneracy of fundamental frequency

For NA ≠ 0 (max 50)

6th and following NA-1 cards - (Format 4E0.1.11.3)
col 1-18 Atomic weight of atom
col 19-36 X-coordinate of atom (Å)
col 37-54 Y-coordinate of atom (Å)
col 55-72 Z-coordinate of atom (Å)

Next card (Format E0.1.11.3)
col 1-18 Go E Statistical weight of the 0th state
Note: This is the last card if NUM = 0.

Following cards - (Format 2E0.1.11.3)
col 1-18 Fundamental frequency (1/cm)
col 19-36 Degeneracy of fundamental frequency

INPUT FOR ONE DEBYE THETA SOLID

3rd card - (Format E0.1.11.3)
col 1-18 Debye theta ($^{\circ}$ K)

4th card - (Format 2E0.1.11.3)
col 1-18 Number of atoms per unit cell
col 19-36 Dimension (1, 2, or 3)

5th card - (Format 3E0.1.11.3)
col 1-18 Initial temperature ($^{\circ}$ K)
col 19-36 Temperature increment ($^{\circ}$ K)
col 37-54 Final temperature ($^{\circ}$ K)

Note: No more than 1000 temperatures may
be specified.

INPUT FOR TWO DEBYE THETA SOLID

3rd card - (Format 2E0.1.11.3)
col 1-18 Debye theta transverse ($^{\circ}$ K)
col 19-36 Debye theta longitudinal ($^{\circ}$ K)

4th card - (Format E0.1.11.3)
col 1-18 Number of atoms per unit cell

5th card - (Format 3E0.1.11.3)
col 1-18 Initial temperature ($^{\circ}$ K)
col 19-36 Temperature increment ($^{\circ}$ K)
col 37-54 Final temperature ($^{\circ}$ K)

Note: No more than 1000 temperatures may
be specified.

OUTPUT

- On Film
1. The ID card and input parameters.
 2. The 4th degree fits to the thermodynamic functions.
 3. A listing of the values of the thermodynamic functions plus the integration constant for the range of temperatures specified.
 4. The variance of the fit on the entropy and a listing of values computed from the fit.
 5. Graphs of the thermodynamic functions.

Off Line Print - 1, 2, and 3 above.

On Line Print - (Sw 34 on, 37 off) - 1, 2, and 3 above.
(Sw 34 on, 37 on) - Just the ID card.
(Sw 34 off) - Nothing.

Sw 34 and 37 must be set before reading in the data for the case to be listed.

The following are seven cases illustrating
the input and film output of STRETCH TDF.

		<u>Page</u>
Case one	Monoatomic S Sulfur	12
Case two	Diatomic PO Phosphorus Oxide	20
Case three	Linear Polyatomic AlFO	28
Case four	Non-Linear Polyatomic CF ₄ Carbon tetrafluoride	36
Case five	Polyatomic with Moment of Inertia Li ₂ O	44
Case six	One Debye Theta Solid B Boron	52
Case seven	Two Debye Theta Solid BN Boron Nitride	61

GMX-2 LOADING FORM FOR STRETCH

PROGRAMMER:

PROBLEM: TDF

DATE:

PAGE

OF

±X.XX	±EEE	±X.XX	±EEE	±X.XX	±EEE	±X.XX	±EEE	Card no.
1	5	19	33	37	51	55	69	73
MONAHTONIC	S		SULFUR			CASE ONE		1
CC01								2
+3.2066	+CC1							3
+3.	+CC2+1.		+CC2+6.		+CC3			4
+5.	+CC0 CC03							5
+3.968	+CC2+3.		+CC0					6
+5.736	+CC2+1.		+CC0					7
+9.239	+CC3+5.		+CC0					8

-12-

MONOATOMIC S SULFUR CASE ONE

MOLECULAR WT GO E MONOATOMIC
5.2066000000+001 5.0000000000+000

TERM VALUE 1/CM STAT WT
5.9880000000+002 5.0000000000+000
5.7360000000+002 1.0000000000+000
9.2390000000+003 5.0000000000+000

FO-HO/T = -3.20658760548+001 -1.27095526502-002T 4.43271817537-006T^2 -7.66582647852-010T^3 4.92952632247-014T^4

H-HO = -2.37197073675-003 5.55964933146-003T -3.09577627181-007T^2 8.08186445297-011T^3 -6.02949143944-015T^4

SO = 3.75363760171+001 1.25604911165-002T -4.44106000037-006T^2 7.79763397882-010T^3 -5.07037247009-014T^4

TEMP (DEG K)	FO-HO/T (C/M/D)	HO (KC/M)	SO (C/M/D)	IC
5.00000000+02	-3.47813107+01	1.60146243+00	4.01195188+01	1.11154091+03
4.00000000+02	-3.63279922+01	2.16247677+00	4.17341841+01	1.33256662+03
5.00000000+02	-3.75368577+01	2.71181853+00	4.29604948+01	1.47656167+03
6.00000000+02	-3.85253762+01	3.25038572+00	4.39426897+01	1.55637115+03
7.00000000+02	-3.93592914+01	3.78049748+00	4.47600021+01	1.58510108+03
8.00000000+02	-4.00791423+01	4.30420722+00	4.54594013+01	1.57448027+03
9.00000000+02	-4.07116159+01	4.82307501+00	4.60705882+01	1.53468126+03
1.00000000+03	-4.12751590+01	5.33825022+00	4.66134092+01	1.47445181+03
1.10000000+03	-4.17830218+01	5.85059042+00	4.71017404+01	1.40128233+03
1.20000000+03	-4.22450245+01	6.36075922+00	4.75456572+01	1.32155246+03
1.30000000+03	-4.26686374+01	6.86929647+00	4.79527116+01	1.24064997+03
1.40000000+03	-4.30596700+01	7.37666467+00	4.83287162+01	1.16306575+03
1.50000000+03	-4.34227268+01	7.88327707+00	4.86782449+01	1.09247072+03
1.60000000+03	-4.37615171+01	8.38951292+00	4.90049627+01	1.03177963+03
1.70000000+03	-4.40790720+01	8.89572406+00	4.93118509+01	9.83206415+02
1.80000000+03	-4.4378994+01	9.40223650+00	4.96013641+01	9.48314390+02
1.90000000+03	-4.46600971+01	9.90934939+00	4.98755441+01	9.28063917+02
2.00000000+03	-4.49274370+01	1.04173330+01	5.01361035+01	9.22859111+02
2.10000000+03	-4.51814284+01	1.09264269+01	5.03844888+01	9.32594626+02
2.20000000+03	-4.54233669+01	1.14368388+01	5.06219300+01	9.56703064+02
2.30000000+03	-4.56543722+01	1.19487437+01	5.08494781+01	9.94203193+02
2.40000000+03	-4.58754180+01	1.24622847+01	5.10680367+01	1.04374901+03
2.50000000+03	-4.60873559+01	1.29775741+01	5.12783855+01	1.10367952+03
2.60000000+03	-4.62909344+01	1.34946946+01	5.14812015+01	1.17206915+03
2.70000000+03	-4.64868143+01	1.40137021+01	5.16770744+01	1.24677856+03
2.80000000+03	-4.66755822+01	1.45346277+01	5.18665206+01	1.32550573+03
2.90000000+03	-4.68577599+01	1.50574807+01	5.20499947+01	1.40883725+03
3.00000000+03	-4.70338145+01	1.55822505+01	5.22278980+01	1.48529959+03
3.10000000+03	-4.72041644+01	1.61089100+01	5.24005870+01	1.56141037+03
3.20000000+03	-4.73691867+01	1.66374176+01	5.25683797+01	1.63172949+03
3.30000000+03	-4.75292218+01	1.71677195+01	5.27315611+01	1.69391021+03
3.40000000+03	-4.76845778+01	1.76997523+01	5.28903873+01	1.74574987+03
3.50000000+03	-4.78355349+01	1.82334443+01	5.30450904+01	1.78524065+03
3.60000000+03	-4.79823479+01	1.87687178+01	5.31958806+01	1.81061994+03
3.70000000+03	-4.81252498+01	1.93054908+01	5.33429500+01	1.82420600+03
3.80000000+03	-4.82644537+01	1.98436775+01	5.34864741+01	1.81352106+03
3.90000000+03	-4.84001554+01	2.03831907+01	5.36266146+01	1.78919518+03
4.00000000+03	-4.85325348+01	2.09239419+01	5.37635203+01	1.74716197+03
4.10000000+03	-4.86617578+01	2.14658427+01	5.38973292+01	1.68763515+03



4.20000000+03	-4.87879777+01	2.20088052+01	5.40281694+01	1.61137258+03
4.30000000+03	-4.89113363+01	2.25527431+01	5.41561602+01	1.51972557+03
4.40000000+03	-4.90319632+01	2.30975717+01	5.42814133+01	1.41468806+03
4.50000000+03	-4.91499868+01	2.36432087+01	5.44040332+01	1.29894572+03
4.60000000+03	-4.92655150+01	2.41895742+01	5.45241181+01	1.17592493+03
4.70000000+03	-4.93786560+01	2.47365913+01	5.46417605+01	1.04984172+03
4.80000000+03	-4.94895089+01	2.52841861+01	5.47570477+01	9.25750658+02
4.90000000+03	-4.95981667+01	2.58322876+01	5.48700621+01	8.09593613+02
5.00000000+03	-4.97047184+01	2.63808285+01	5.49808821+01	7.08248540+02
5.10000000+03	-4.98092397+01	2.69297442+01	5.50895817+01	6.29578187+02
5.20000000+03	-4.99118135+01	2.74789738+01	5.51962315+01	5.82478786+02
5.30000000+03	-5.00125099+01	2.80284595+01	5.53008895+01	5.76928700+02
5.40000000+03	-5.01113974+01	2.85781467+01	5.54036487+01	6.24037059+02
5.50000000+03	-5.02085400+01	2.91279840+01	5.55045371+01	7.36092373+02
5.60000000+03	-5.03039988+01	2.96779229+01	5.56036279+01	9.26611125+02
5.70000000+03	-5.03978312+01	3.02279182+01	5.57000947+01	1.21038636+03
5.80000000+03	-5.04900917+01	3.07779273+01	5.57966309+01	1.60353627+03
5.90000000+03	-5.05808321+01	3.13279104+01	5.58906474+01	2.12355275+03
6.00000000+03	-5.06701014+01	3.18778306+01	5.59830731+01	2.78934996+03

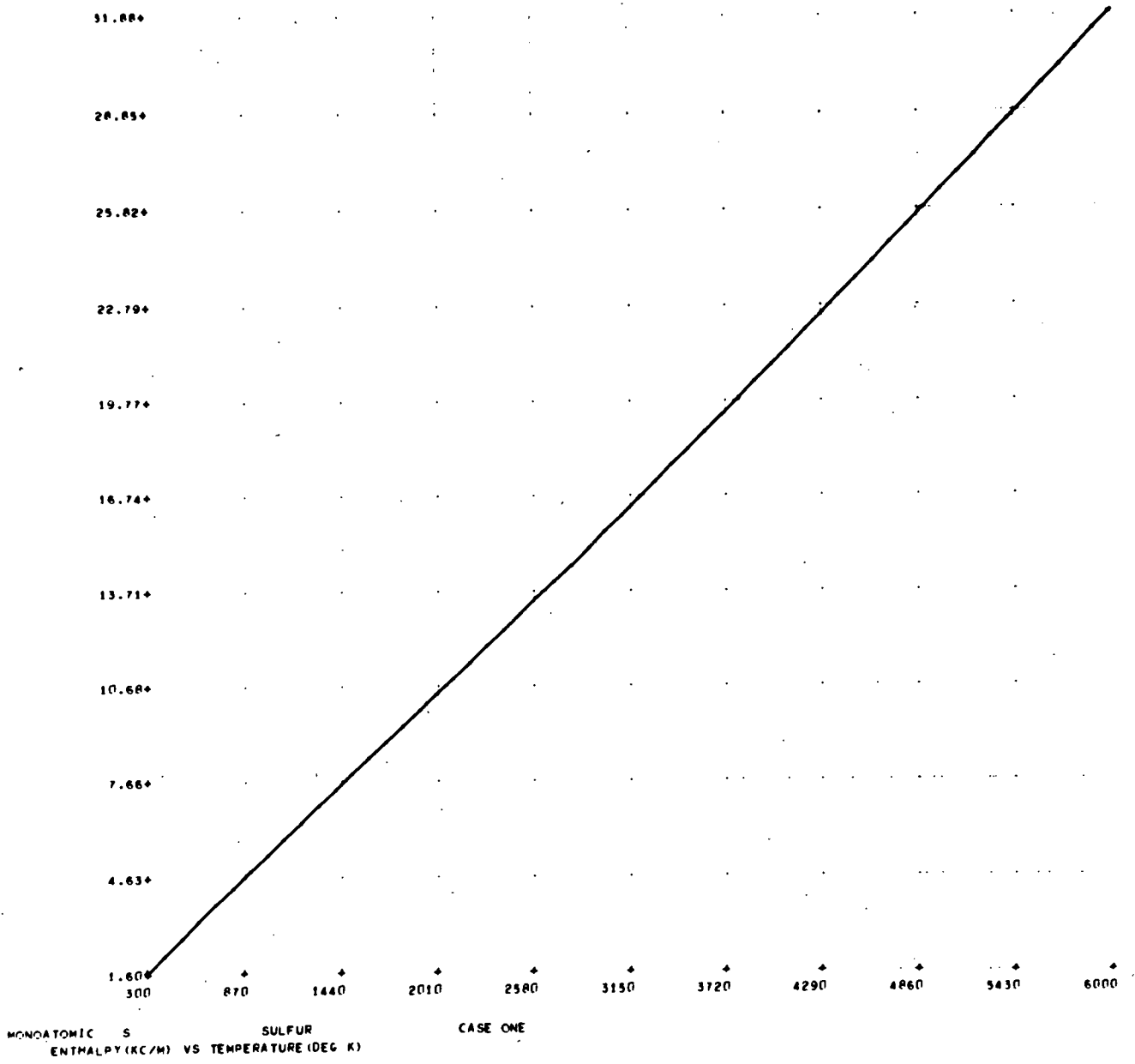
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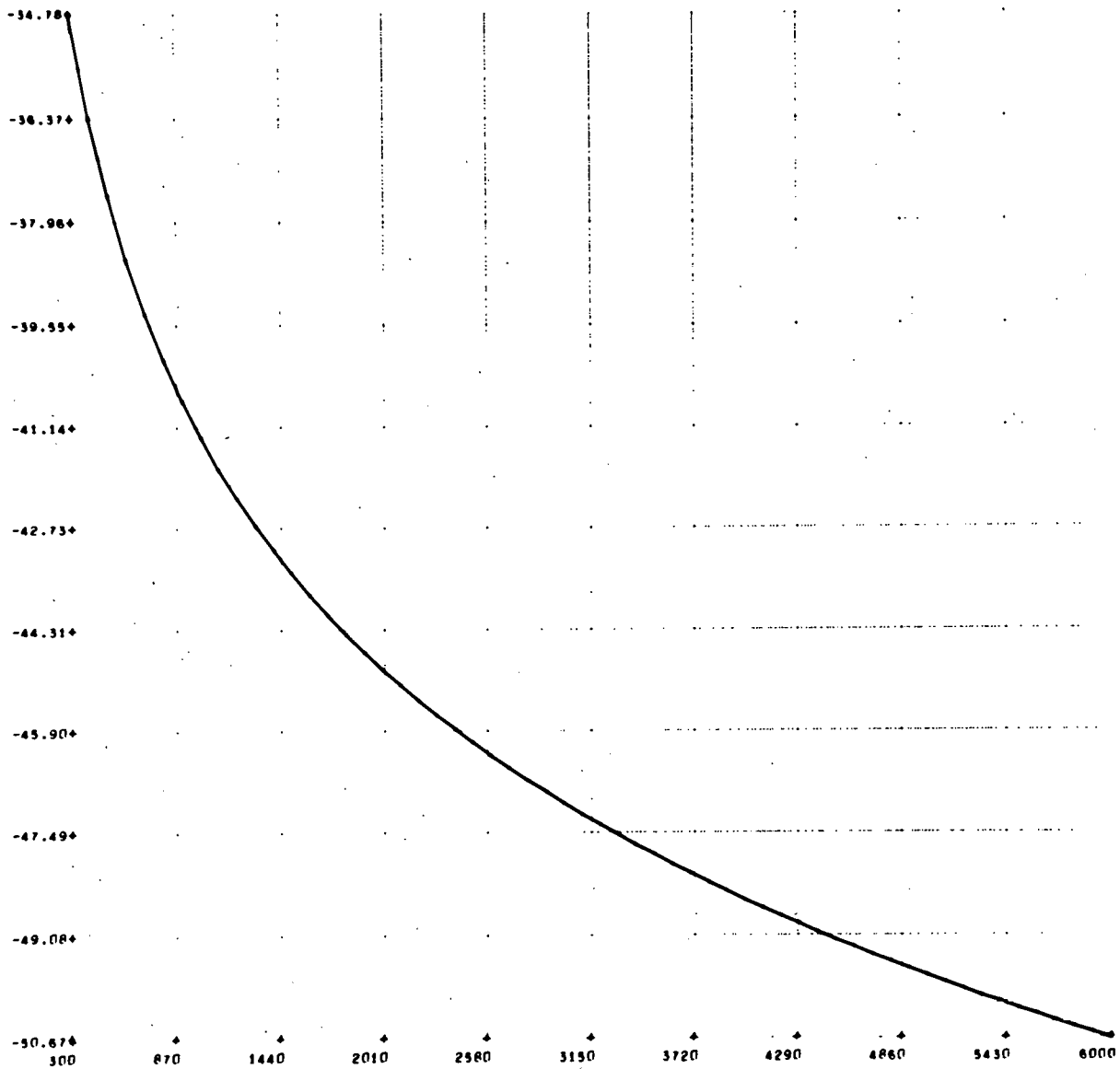
VARIANCE
3.43552964957-002

TEMP (DEG K)	S0	S0 FROM FIT
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4.00000000+02	4.17341841+01	4.18986097+01
5.00000000+02	4.29604948+01	4.28006580+01
6.00000000+02	4.39426857+01	4.36357467+01
7.00000000+02	4.47600021+01	4.44078852+01
8.00000000+02	4.54594013+01	4.51209811+01
9.00000000+02	4.60705882+01	4.57787402+01
1.00000000+03	4.66134092+01	4.63848667+01
1.10000000+03	4.71017404+01	4.69428633+01
1.20000000+03	4.75456572+01	4.74561307+01
1.30000000+03	4.79527116+01	4.79279482+01
1.40000000+03	4.83287162+01	4.83614732+01
1.50000000+03	4.86782449+01	4.87597414+01
1.60000000+03	4.90049627+01	4.91256669+01
1.70000000+03	4.93118509+01	4.94620423+01
1.80000000+03	4.96013641+01	4.97715381+01
1.90000000+03	4.98755441+01	5.00567034+01
2.00000000+03	5.01361035+01	5.03199655+01
2.10000000+03	5.03844888+01	5.05636301+01
2.20000000+03	5.06219300+01	5.07898812+01
2.30000000+03	5.08494781+01	5.10007809+01
2.40000000+03	5.10680367+01	5.11982699+01
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2.70000000+03	5.16770744+01	5.17278532+01
2.80000000+03	5.18665206+01	5.18886714+01
2.90000000+03	5.20499947+01	5.20439564+01
3.00000000+03	5.22278980+01	5.21949187+01
3.10000000+03	5.24005870+01	5.23426470+01
3.20000000+03	5.25683797+01	5.24881085+01
3.30000000+03	5.27315611+01	5.26321485+01
3.40000000+03	5.28903873+01	5.27754906+01
3.50000000+03	5.30450904+01	5.29187369+01
3.60000000+03	5.31958806+01	5.30623678+01
3.70000000+03	5.33429500+01	5.32067417+01
3.80000000+03	5.34864741+01	5.33520957+01
3.90000000+03	5.36266146+01	5.34985450+01
4.00000000+03	5.37635203+01	5.36460831+01
4.10000000+03	5.38973292+01	5.37945820+01
4.20000000+03	5.40281694+01	5.39437918+01
4.30000000+03	5.41561602+01	5.40933409+01
4.40000000+03	5.42814133+01	5.42427363+01
4.50000000+03	5.44040332+01	5.43913629+01
4.60000000+03	5.45241181+01	5.45384843+01
4.70000000+03	5.46417605+01	5.46832421+01
4.80000000+03	5.47570477+01	5.48246565+01
4.90000000+03	5.48700621+01	5.49616257+01
5.00000000+03	5.49808821+01	5.50929264+01
5.10000000+03	5.50895817+01	5.52172136+01
5.20000000+03	5.51962315+01	5.53330206+01
5.30000000+03	5.53008985+01	5.54387590+01
5.40000000+03	5.54036487+01	5.55327187+01
5.50000000+03	5.55045371+01	5.56130680+01

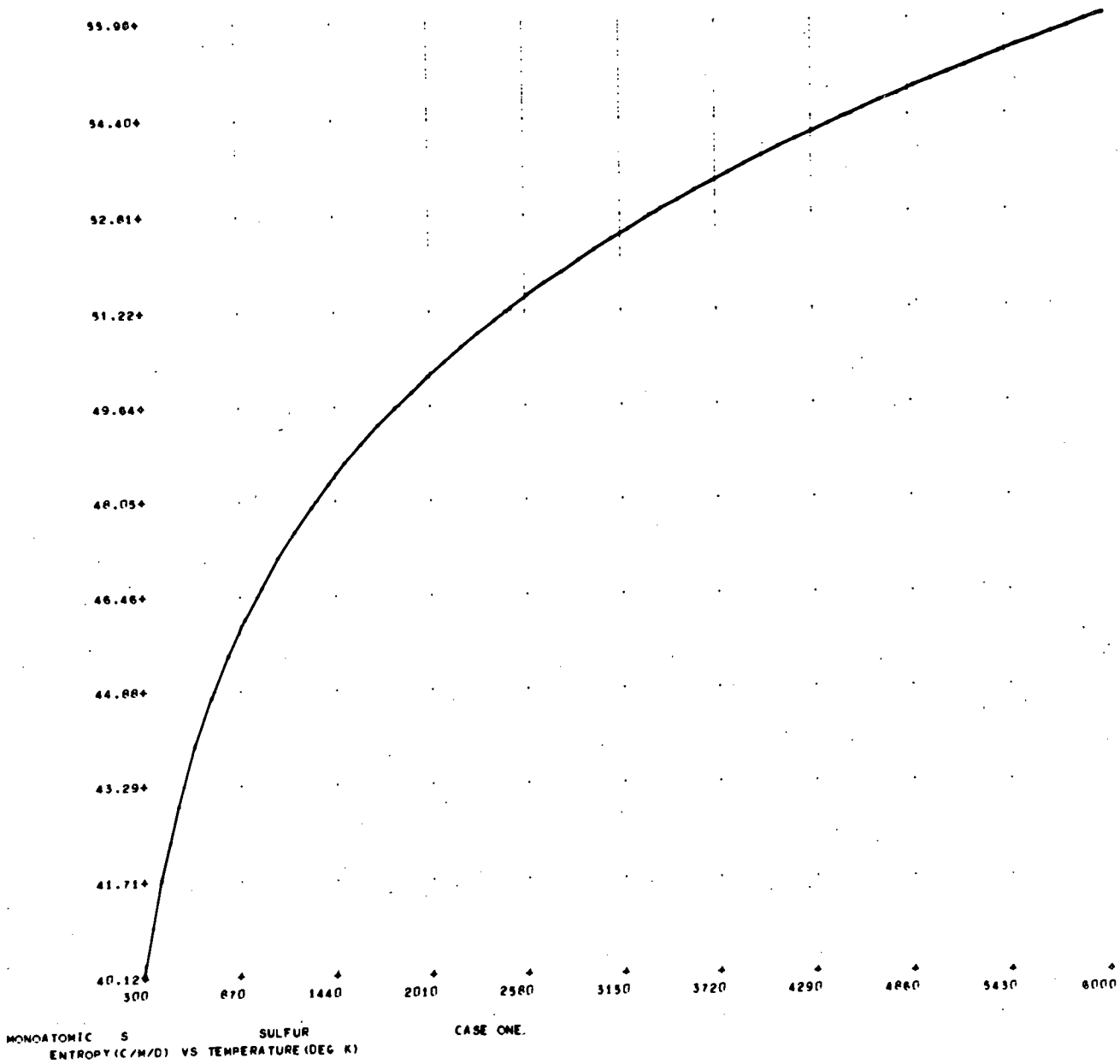


5.6000000+03	5.56036279+01	5.56778533+01
5.7000000+03	5.57009747+01	5.57249994+01
5.8000000+03	5.57966309+01	5.57523097+01
5.9000000+03	5.58906474+01	5.57574855+01
6.0000000+03	5.59830731+01	5.57580266+01





MONOATOMIC S SULFUR CASE ONE
 FREE ENERGY (C/M/D) VS TEMPERATURE (DEG K)



GMX-2 LOADING FORM FOR STRETCH

PROGRAMMER:

PROBLEM: TDF

DATE:

PAGE

OF

±X.XX	±EEE	±X.XX	±EEE	±X.XX	±EEE	±X.XX	±EEE	OF
1	5	19	33	37	51	55	69	73
DIATOMIC Pd			PHOSPHORUS & XIDE			CASE TUD		1
CCC2								2
+4.6975	+0.01	+1.	+0.00					3
+3.	+0.02	+1.	+0.02	+6.	+0.03			4
+1.23064	+0.03	+6.52	+0.00	+7.629	-0.01	+5.5	-0.03	5
+2.	+0.00	0.001						6
+2.238	+0.02	+2.	+0.00					7

-20-

DIATOMIC PO PHOSPHORUS OXIDE CASE TWO

MOLECULAR WT 4.6975000000+001
 SYMMETRY NO. 1.0000000000+000

W E 1.2500400000+003
 WE XE 6.5200000000+000
 B E 7.6290000000+001
 A E 5.5000000000+003

CO E 2.0000000000+000

TERM VALUE 1/CM 2.2500000000+002
 STAT WT 2.0000000000+000

FO-MO/T = -4.17653409226+001 -1.78434348953+002T 5.91502790787+006T^2 -1.00435169991+009T^3 6.40751973377+014T^4

M-MO = -1.74072446396+001 7.73774558639+003T 5.19572783835+007T^2 -8.92101803862+011T^3 5.83702582486+015T^4

SO = 4.89614474922+001 1.88681789769+002T -6.19986382930+006T^2 1.04349052900+009T^3 -6.61365504407+014T^4

TEMP (DEG K)	FO-MO/T (C/M/D)	MO (K/C/M)	SO (C/M/D)	IC
3.0000000+02	-4.56539453+01	2.26031271+00	5.31883210+01	1.51663157+03
4.0000000+02	-4.78248166+01	3.02520041+00	5.53878177+01	1.76078039+03
5.0000000+02	-4.95177988+01	3.80833141+00	5.71344616+01	1.91920415+03
6.0000000+02	-5.09124953+01	4.61185890+00	5.85989268+01	2.01105402+03
7.0000000+02	-5.21029926+01	5.43315585+00	5.98646438+01	2.04914009+03
8.0000000+02	-5.31443024+01	6.26881026+00	6.09803152+01	2.04599018+03
9.0000000+02	-5.40713666+01	7.11583053+00	6.19778449+01	2.00511864+03
1.0000000+03	-5.49078276+01	7.97185529+00	6.28796829+01	1.94129970+03
1.1000000+03	-5.56704842+01	8.83508209+00	6.37023770+01	1.86055964+03
1.2000000+03	-5.63717399+01	9.70414508+00	6.44585275+01	1.77011800+03
1.3000000+03	-5.70210384+01	1.05780055+01	6.51579657+01	1.67634144+03
1.4000000+03	-5.76257521+01	1.14558664+01	6.58085138+01	1.58472220+03
1.5000000+03	-5.81917567+01	1.23371101+01	6.64164968+01	1.49987880+03
1.6000000+03	-5.87238171+01	1.32212526+01	6.69870999+01	1.42557392+03
1.7000000+03	-5.92258549+01	1.41079102+01	6.75246255+01	1.36474483+03
1.8000000+03	-5.97011393+01	1.49967757+01	6.80326813+01	1.31954279+03
1.9000000+03	-6.01524260+01	1.58876008+01	6.85143212+01	1.29137885+03
2.0000000+03	-6.05820609+01	1.67801824+01	6.89721521+01	1.28097423+03
2.1000000+03	-6.09920578+01	1.76743536+01	6.94084167+01	1.28841398+03
2.2000000+03	-6.13841596+01	1.85699757+01	6.98250577+01	1.31320302+03
2.3000000+03	-6.17598850+01	1.94669325+01	7.02237687+01	1.35432396+03
2.4000000+03	-6.21205654+01	2.03651263+01	7.06060347+01	1.41029621+03
2.5000000+03	-6.24673752+01	2.12644740+01	7.09731648+01	1.47923603+03
2.6000000+03	-6.28013555+01	2.21649050+01	7.13263189+01	1.55891735+03
2.7000000+03	-6.31234335+01	2.30663584+01	7.16665292+01	1.64883313+03
2.8000000+03	-6.34344391+01	2.39687818+01	7.19947183+01	1.74025714+03
2.9000000+03	-6.37351176+01	2.48721298+01	7.23117141+01	1.83630608+03
3.0000000+03	-6.40261414+01	2.57763627+01	7.26182623+01	1.93200200+03
3.1000000+03	-6.43081187+01	2.66814459+01	7.29150367+01	2.0283381+03
3.2000000+03	-6.45816019+01	2.75873488+01	7.32026884+01	2.1102510+03
3.3000000+03	-6.48470941+01	2.84940446+01	7.34816531+01	2.18788699+03
3.4000000+03	-6.51050549+01	2.94015095+01	7.37525577+01	2.25189108+03



3.50000000+03	-6.53559051+01	3.03097224+01	7.40150250+01	2.30222759+03
3.60000000+03	-6.56000410+01	3.12106644+01	7.42710022+01	2.33506940+03
3.70000000+03	-6.58377003+01	3.21203105+01	7.45211177+01	2.35093533+03
3.80000000+03	-6.60695052+01	3.30300697+01	7.47630020+01	2.34595330+03
3.90000000+03	-6.62954000+01	3.39497005+01	7.50000537+01	2.31992366+03
4.00000000+03	-6.65160000+01	3.40614103+01	7.52313609+01	2.27230000+03
4.10000000+03	-6.67313362+01	3.57737763+01	7.54566475+01	2.20300000+03
4.20000000+03	-6.69417112+01	3.66067924+01	7.56766617+01	2.11390000+03
4.30000000+03	-6.71473500+01	3.76004493+01	7.58916495+01	2.00541591+03
4.40000000+03	-6.73400000+01	3.85147307+01	7.61010000+01	1.00012000+03
4.50000000+03	-6.75453019+01	3.94296532+01	7.63074471+01	1.74120000+03
4.60000000+03	-6.77537000+01	4.03451000+01	7.65000000+01	1.59200000+03
4.70000000+03	-6.79266921+01	4.12613200+01	7.67000000+01	1.44000000+03
4.80000000+03	-6.81110000+01	4.21700000+01	7.69000000+01	1.20000000+03
4.90000000+03	-6.82920000+01	4.30954302+01	7.70000000+01	1.14665973+03
5.00000000+03	-6.84706300+01	4.40133761+01	7.72733060+01	1.02164000+03
5.10000000+03	-6.86450212+01	4.49319130+01	7.74552002+01	9.23500000+02
5.20000000+03	-6.88161692+01	4.58510367+01	7.76356763+01	8.63137331+02
5.30000000+03	-6.89841951+01	4.67707432+01	7.78000000+01	8.52015000+02
5.40000000+03	-6.91492124+01	4.76910200+01	7.79000000+01	9.06230000+02
5.50000000+03	-6.93113200+01	4.86110000+01	7.81490000+01	1.03000000+03
5.60000000+03	-6.94706464+01	4.95333200+01	7.83150000+01	1.26654416+03
5.70000000+03	-6.96272616+01	5.04553200+01	7.84790000+01	1.60000000+03
5.80000000+03	-6.97812661+01	5.13790000+01	7.86395200+01	2.00000000+03
5.90000000+03	-6.99327471+01	5.23010364+01	7.87973295+01	2.71626124+03
6.00000000+03	-7.00817073+01	5.32247307+01	7.89525765+01	3.52736329+03

ENTROPY FIT

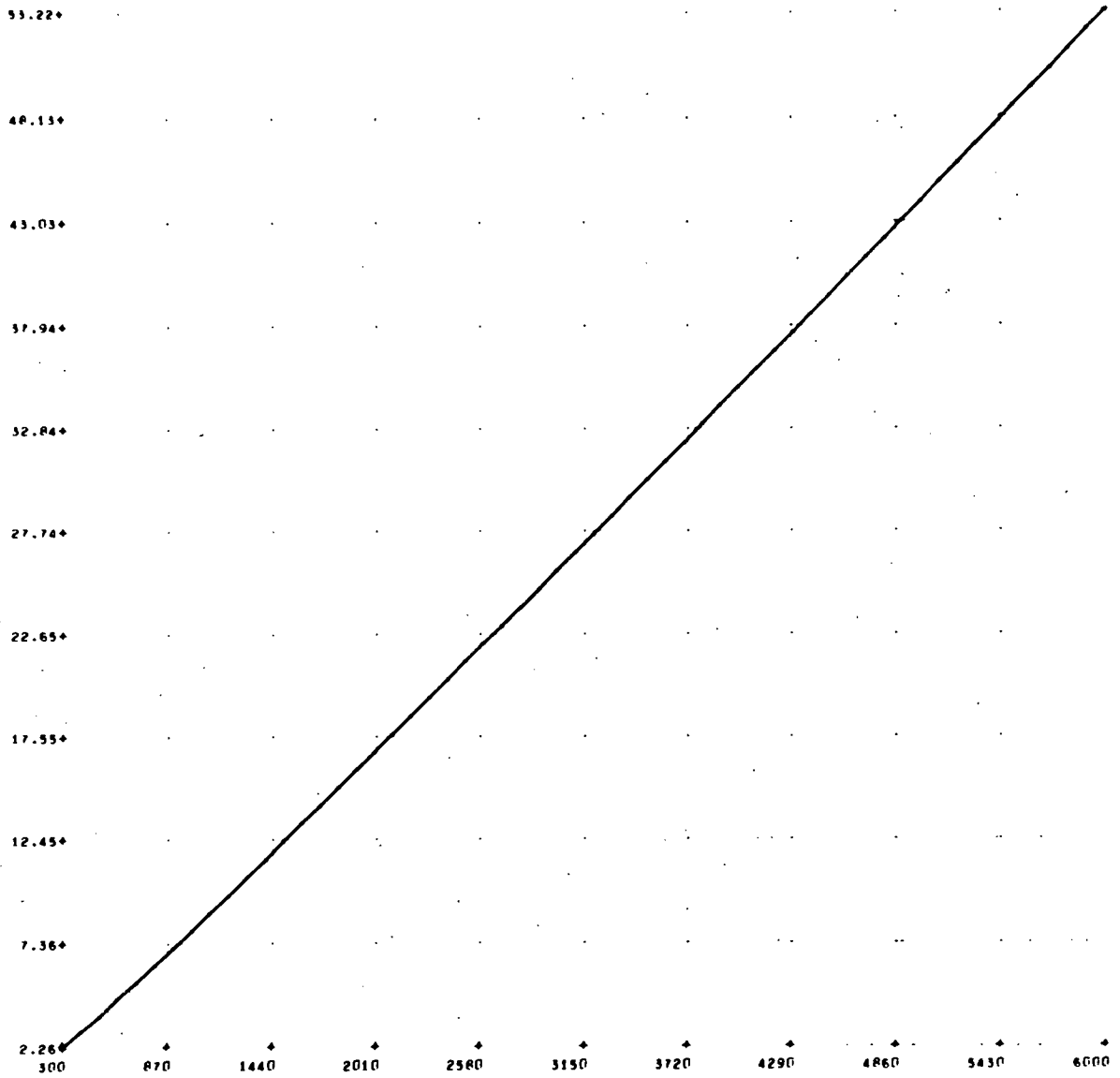
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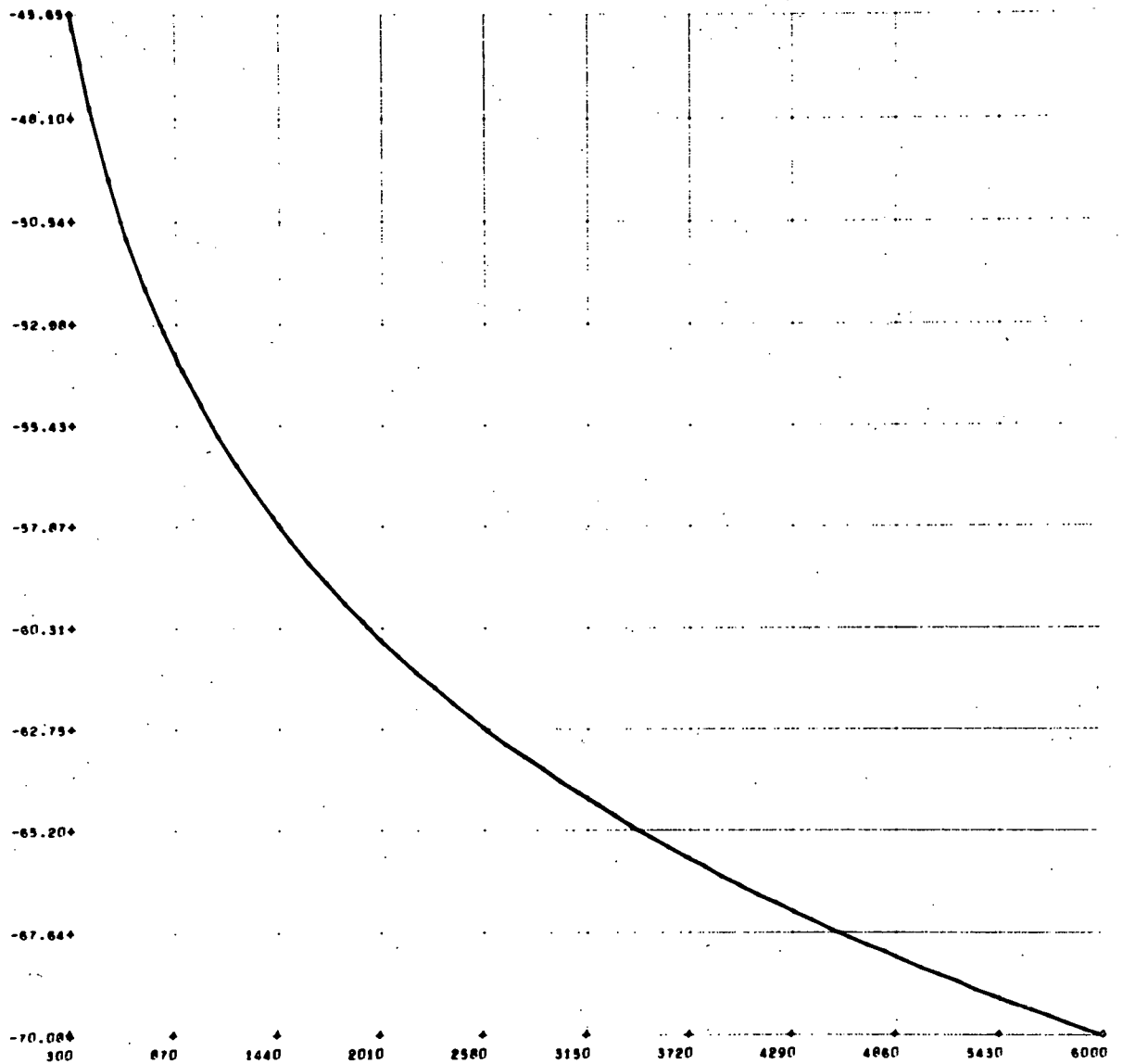
TEMP (DEG K)	SO	SO FROM FIT
3.00000000+02	5.31883210+01	5.40915520+01
4.00000000+02	5.53878177+01	5.55818312+01
5.00000000+02	5.71344616+01	5.69718738+01
6.00000000+02	5.85989268+01	5.82672266+01
7.00000000+02	5.98646438+01	5.94732774+01
8.00000000+02	6.09803132+01	6.05932554+01
9.00000000+02	6.19784449+01	6.16382313+01
1.00000000+03	6.28796829+01	6.26071166+01
1.10000000+03	6.37023770+01	6.35066645+01
1.20000000+03	6.44585275+01	6.43414692+01
1.30000000+03	6.51579657+01	6.51159664+01
1.40000000+03	6.58085138+01	6.58344328+01
1.50000000+03	6.64164968+01	6.65009866+01
1.60000000+03	6.69870999+01	6.71195872+01
1.70000000+03	6.75246255+01	6.76940352+01
1.80000000+03	6.80326813+01	6.82279726+01
1.90000000+03	6.85143212+01	6.87248823+01
2.00000000+03	6.89721521+01	6.91880896+01
2.10000000+03	6.94084167+01	6.96207594+01
2.20000000+03	6.98250577+01	7.00258991+01
2.30000000+03	7.02237687+01	7.04063569+01
2.40000000+03	7.06060347+01	7.07648224+01
2.50000000+03	7.09731648+01	7.11038265+01
2.60000000+03	7.13263189+01	7.14257413+01
2.70000000+03	7.16665292+01	7.17327800+01
2.80000000+03	7.19947183+01	7.20269975+01
2.90000000+03	7.23117141+01	7.23102897+01
3.00000000+03	7.26182623+01	7.25843937+01
3.10000000+03	7.29150367+01	7.28508880+01
3.20000000+03	7.32026484+01	7.31111923+01
3.30000000+03	7.34816531+01	7.33665678+01
3.40000000+03	7.37525577+01	7.36181166+01
3.50000000+03	7.40158258+01	7.38667823+01
3.60000000+03	7.42718822+01	7.41133499+01
3.70000000+03	7.45211177+01	7.43584453+01
3.80000000+03	7.47638920+01	7.46025360+01
3.90000000+03	7.50000537+01	7.48459306+01
4.00000000+03	7.52313609+01	7.50887791+01
4.10000000+03	7.54566475+01	7.53310726+01
4.20000000+03	7.56766617+01	7.55726436+01
4.30000000+03	7.58916495+01	7.58131659+01
4.40000000+03	7.61018399+01	7.60521545+01
4.50000000+03	7.63074471+01	7.62889656+01
4.60000000+03	7.65086709+01	7.65227968+01
4.70000000+03	7.67056985+01	7.67526870+01
4.80000000+03	7.68987054+01	7.69775163+01
4.90000000+03	7.70878563+01	7.71960060+01
5.00000000+03	7.72733060+01	7.74067187+01
5.10000000+03	7.74552002+01	7.76080585+01
5.20000000+03	7.76336763+01	7.77982705+01
5.30000000+03	7.78088636+01	7.79754411+01
5.40000000+03	7.79808844+01	7.81337498+01
5.50000000+03	7.81498545+01	7.82822106+01



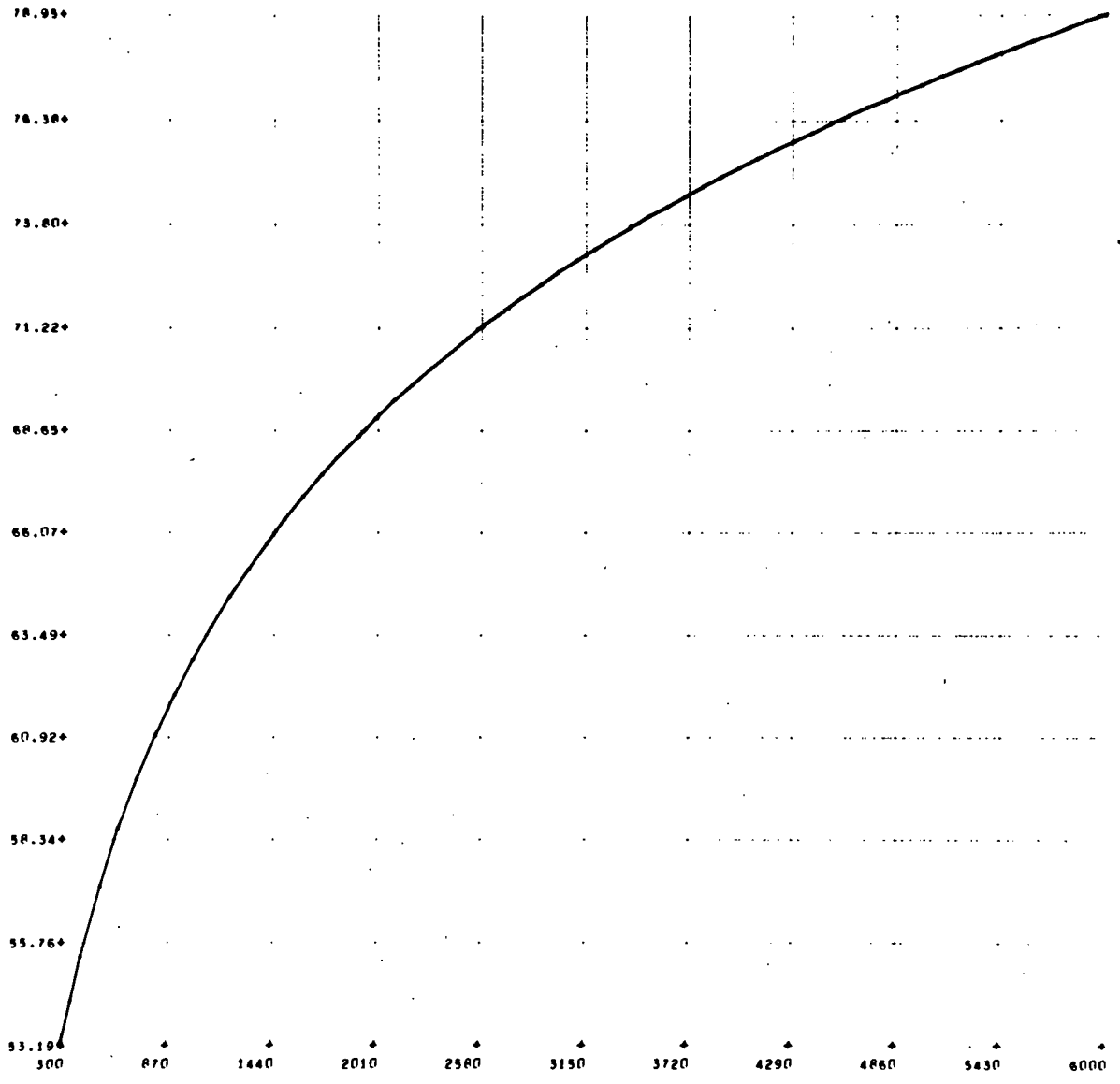
5.6000000+03	7.83158830+01	7.84071887+01
5.7000000+03	7.84790757+01	7.85098841+01
5.8000000+03	7.86395248+01	7.85875896+01
5.9000000+03	7.87975295+01	7.86374592+01
6.0000000+03	7.89525765+01	7.86564884+01



DIATOMIC PO PHOSPHORUS OXIDE CASE TWO
ENTHALPY (KCAL/M) VS TEMPERATURE (DEG K)



DIATOMIC PO PHOSPHORUS OXIDE CASE TWO
FREE ENERGY (C/M/D) VS TEMPERATURE (DEG. K)



DIATOMIC PO PHOSPHORUS OXIDE CASE TWO
ENTROPY (C/M/D) VS TEMPERATURE (DEG K)

GMX-2 LOADING FORM FOR STRETCH

PROGRAMMER:

PROBLEM: *TDF*

DATE:

PAGE

OF

±X.XX	±EEE	±X.XX	±EEE	±X.XX	±EEE	±X.XX	±EEE	OF
1	15	19	33	37	51	55	69	73
<i>LINEAR POLYATOMIS</i>		<i>ALFD</i>				<i>CASE THREE</i>		
<i>0003</i>								<i>1</i>
<i>+6.198</i>	<i>+001</i>	<i>+1.</i>	<i>+000</i>					<i>2</i>
<i>+3.</i>	<i>+002</i>	<i>+1.</i>	<i>+002</i>	<i>+6.</i>	<i>+003</i>			<i>3</i>
<i>0000 0000 0003</i>								<i>4</i>
<i>+1.548</i>	<i>+091</i>							<i>5</i>
<i>+1.</i>	<i>+000</i>							<i>6</i>
<i>+9.</i>	<i>+002</i>	<i>+1.</i>	<i>+000</i>					<i>7</i>
<i>+7.5</i>	<i>+002</i>	<i>+1.</i>	<i>+000</i>					<i>8</i>
<i>+5.</i>	<i>+002</i>	<i>+2.</i>	<i>+000</i>					<i>9</i>
								<i>10</i>

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LINEAR POLYATOMIC ALFO

CASE THREE

MOLECULAR WT
6.1900000000+001

SYMMETRY NO.
1.0000000000+000

POLYATOMIC

INERTIA A 10*59
1.5400000000+001

INERTIA B 10*59
0.0000000000+000

INERTIA C 10*59
0.0000000000+000

LINEAR

CO E
1.0000000000+000

VIB FREQ 1/CM
9.0000000000+002
7.5000000000+002
5.0000000000+002

DEGENERACY
1.0000000000+000
1.0000000000+000
2.0000000000+000

FO-HO/T = -4.22468429540+001 -2.32752415291-002T 6.99762690364-006T#2 -1.13135540774-009T#3 7.01675995568-014T#4

H-HO = -1.63324172517+000 1.26252770785-002T 9.87124073742-007T#2 -1.84363664706-010T#3 1.23253608575-014T#4

SO = 4.89007401706+001 3.06732734511-002T -9.95829426012-006T#2 1.66013732241-009T#3 -1.04541428709-013T#4

TEMP (DEG K)	FO-HO/T (C/M/D)	HO (KC/M)	SO (C/M/D)	IC
3.0000000+02	-4.78255338+01	2.46764738+00	5.60510251+01	1.25671727+03
4.0000000+02	-5.03031682+01	3.60931781+00	5.93264627+01	1.54932492+03
5.0000000+02	-5.23928157+01	4.8553740+00	6.21038905+01	1.77603067+03
6.0000000+02	-5.42154223+01	6.16870932+00	6.44966045+01	1.92665244+03
7.0000000+02	-5.58367246+01	7.52586502+00	6.65879603+01	2.00314997+03
8.0000000+02	-5.72889992+01	8.91297182+00	6.84398140+01	2.01403281+03
9.0000000+02	-5.86302619+01	1.03212024+01	7.00982645+01	1.97073014+03
1.0000000+03	-5.98532527+01	1.17448060+01	7.15980586+01	1.88562222+03
1.1000000+03	-6.09840468+01	1.31799067+01	7.29657802+01	1.77063943+03
1.2000000+03	-6.20355832+01	1.46238112+01	7.42220925+01	1.63726975+03
1.3000000+03	-6.30182336+01	1.60745958+01	7.53833072+01	1.49564674+03
1.4000000+03	-6.39404497+01	1.75308533+01	7.64624878+01	1.35469644+03
1.5000000+03	-6.48092148+01	1.89915323+01	7.74702364+01	1.22201708+03
1.6000000+03	-6.56303673+01	2.04558324+01	7.84152625+01	1.10387466+03
1.7000000+03	-6.64088390+01	2.19231338+01	7.93048001+01	1.00523318+03
1.8000000+03	-6.71488341+01	2.33929500+01	8.01449174+01	9.29807034+02
1.9000000+03	-6.78539656+01	2.48648934+01	8.09407515+01	8.80127720+02
2.0000000+03	-6.85273612+01	2.63386518+01	8.16966871+01	8.57620296+02
2.1000000+03	-6.91717468+01	2.78139710+01	8.24164949+01	8.62686360+02
2.2000000+03	-6.97895120+01	2.92906421+01	8.31034402+01	8.94791614+02
2.3000000+03	-7.03827636+01	3.07684915+01	8.37603685+01	9.52556664+02
2.4000000+03	-7.09533679+01	3.22473741+01	8.43897738+01	1.03389014+03
2.5000000+03	-7.15029868+01	3.37271677+01	8.49938539+01	1.13588351+03
2.6000000+03	-7.20310537+01	3.52077684+01	8.55745551+01	1.25330713+03
2.7000000+03	-7.25450580+01	3.66890877+01	8.61336090+01	1.38830725+03
2.8000000+03	-7.30400453+01	3.81710494+01	8.66725629+01	1.53070373+03
2.9000000+03	-7.35191557+01	3.96535876+01	8.71928046+01	1.67808823+03
3.0000000+03	-7.39833686+01	4.11366454+01	8.76955837+01	1.82572295+03
3.1000000+03	-7.44335865+01	4.26201728+01	8.81820293+01	1.96903352+03
3.2000000+03	-7.48702254+01	4.41041262+01	8.86531648+01	2.10333822+03



5.30000000+03	-7.52952339+01	4.55884672+01	8.91099209+01	2.22408778+03
5.40000000+03	-7.57080984+01	4.70731617+01	8.95531460+01	2.32698421+03
5.50000000+03	-7.61098950+01	4.85581798+01	8.99836159+01	2.40805133+03
5.60000000+03	-7.65010712+01	5.00434947+01	9.04020420+01	2.46374013+03
5.70000000+03	-7.68822986+01	5.15290823+01	9.08090776+01	2.49102886+03
5.80000000+03	-7.72540296+01	5.30149214+01	9.12053247+01	2.48752296+03
5.90000000+03	-7.76167253+01	5.45009926+01	9.15913388+01	2.45155510+03
4.00000000+03	-7.79708140+01	5.59872787+01	9.19676337+01	2.38228533+03
4.10000000+03	-7.83166945+01	5.74737640+01	9.23346857+01	2.27980110+03
4.20000000+03	-7.86547381+01	5.89604343+01	9.26929367+01	2.14521754+03
4.30000000+03	-7.89852919+01	6.04472768+01	9.30427981+01	1.98077756+03
4.40000000+03	-7.93086802+01	6.19342799+01	9.33846529+01	1.78995211+03
4.50000000+03	-7.96252068+01	6.34214328+01	9.37188585+01	1.57754038+03
4.60000000+03	-7.99351567+01	6.49087258+01	9.40457492+01	1.34977010+03
4.70000000+03	-8.02387972+01	6.63961500+01	9.43656377+01	1.11439772+03
4.80000000+03	-8.05363801+01	6.78836972+01	9.46788170+01	8.80808775+02
4.90000000+03	-8.08281420+01	6.93713600+01	9.49855624+01	6.60118095+02
5.00000000+03	-8.11143062+01	7.08591314+01	9.52861325+01	4.65270145+02
5.10000000+03	-8.13950833+01	7.23470050+01	9.55807706+01	3.11139307+02
5.20000000+03	-8.16706722+01	7.38349750+01	9.58697058+01	2.14630193+02
5.30000000+03	-8.19412610+01	7.53230360+01	9.61531545+01	1.94777959+02
5.40000000+03	-8.22070278+01	7.68111828+01	9.64313209+01	2.72848624+02
5.50000000+03	-8.24681414+01	7.82994109+01	9.67043979+01	4.72439390+02
5.60000000+03	-8.27247618+01	7.97877158+01	9.69725682+01	8.19578974+02
5.70000000+03	-8.29770410+01	8.12760936+01	9.72360048+01	1.34282794+03
5.80000000+03	-8.32251232+01	8.27645405+01	9.74948716+01	2.07337902+03
5.90000000+03	-8.34691459+01	8.42530529+01	9.77493243+01	3.04515747+03
6.00000000+03	-8.37092396+01	8.57416277+01	9.79995109+01	4.29492139+03

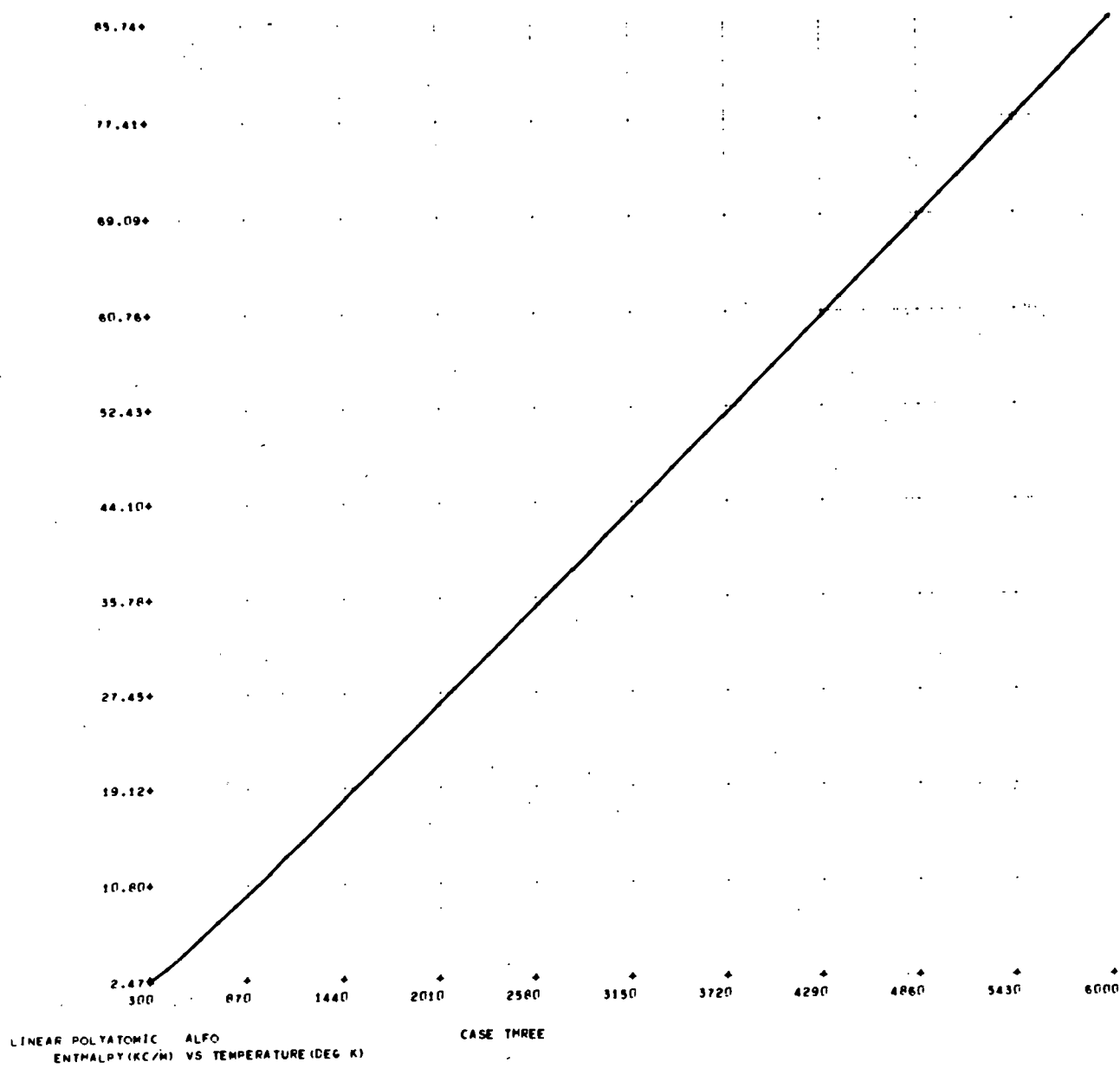
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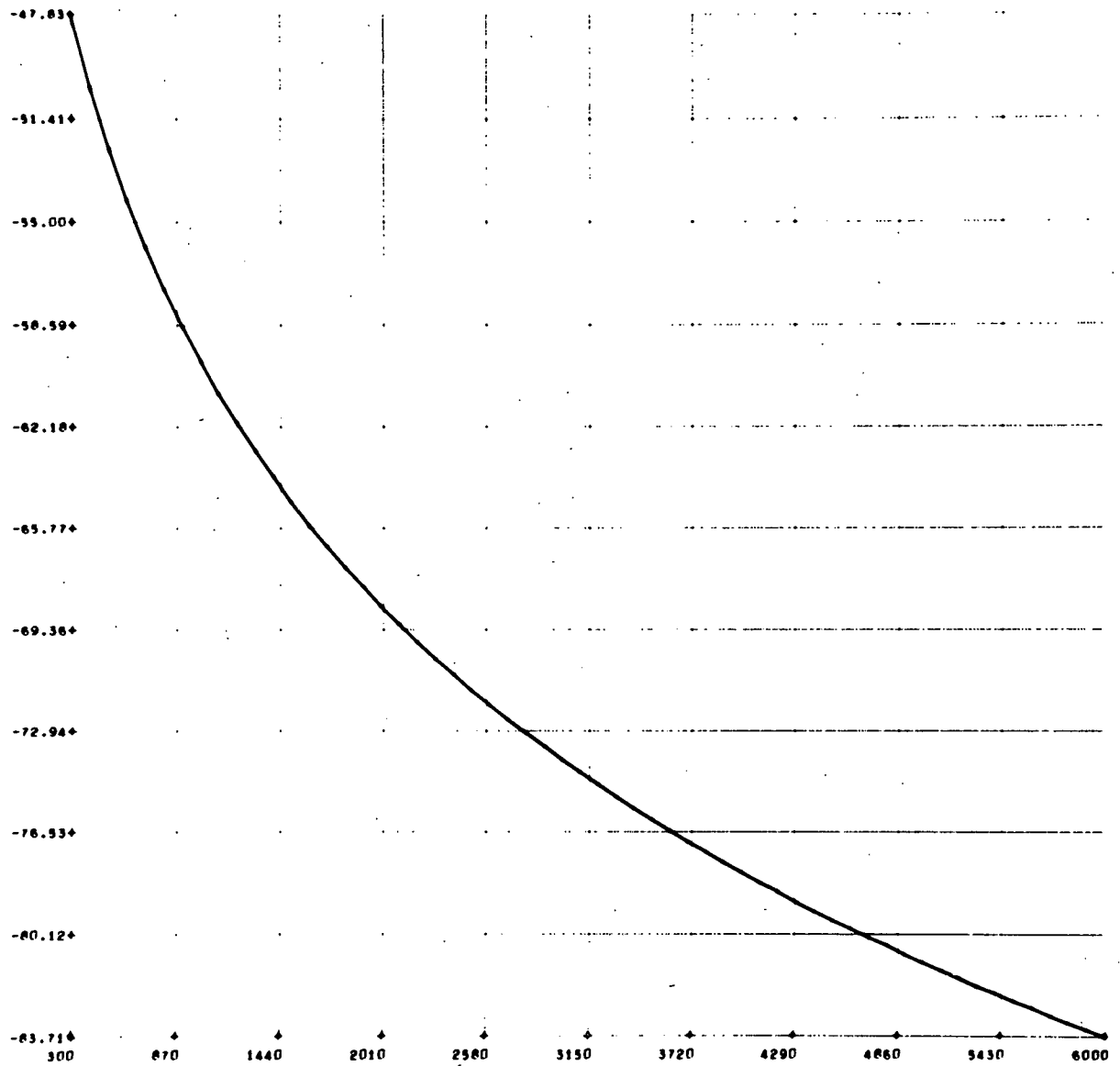
VARIANCE
9.43231836R25--002

TEMP (DEG K)	SO	SO FROM FIT
3.0000000+02	5.60510251+01	5.72504526+01
4.0000000+02	5.93264627+01	5.96R02950+01
5.0000000+02	6.2103R905+01	6.194R7R67+01
6.0000000+02	6.44966045+01	6.40647594+01
7.0000000+02	6.65R79603+01	6.60367941+01
8.0000000+02	6.8439R140+01	6.7R732207+01
9.0000000+02	7.009R2645+01	6.95R211R4+01
1.0000000+03	7.159R05R6+01	7.11713153+01
1.1000000+03	7.29657R02+01	7.264R3R86+01
1.2000000+03	7.42220925+01	7.4020664R+01
1.3000000+03	7.53R33072+01	7.52952193+01
1.4000000+03	7.64624R7R+01	7.647R8767+01
1.5000000+03	7.74702364+01	7.757R2107+01
1.6000000+03	7.84152625+01	7.85995442+01
1.7000000+03	7.9304R001+01	7.954R94R8+01
1.8000000+03	8.01449174+01	8.04322457+01
1.9000000+03	8.09407515+01	8.12550050+01
2.0000000+03	8.16966R71+01	8.2022545R+01
2.1000000+03	8.24164949+01	8.27399363+01
2.2000000+03	8.31034402+01	8.34119941+01
2.3000000+03	8.376036R5+01	8.40432R55+01
2.4000000+03	8.43R9773R+01	8.463R1262+01
2.5000000+03	8.4993R539+01	8.52005R0R+01
2.6000000+03	8.55745551+01	8.57344631+01
2.7000000+03	8.61336090+01	8.62433361+01
2.8000000+03	8.66725629+01	8.67305117+01
2.9000000+03	8.7192R046+01	8.71990510+01
3.0000000+03	8.76955R37+01	8.76517642+01
3.1000000+03	8.81820293+01	8.80912105+01
3.2000000+03	8.86531649+01	8.851969R5+01
3.3000000+03	8.91099209+01	8.89392R55+01
3.4000000+03	8.95531460+01	8.935177R1+01
3.5000000+03	8.99R36159+01	8.975R7321+01
3.6000000+03	9.04020420+01	9.01614523+01
3.7000000+03	9.08090776+01	9.05609925+01
3.8000000+03	9.12053247+01	9.095R1557+01
3.9000000+03	9.159133R8+01	9.13534940+01
4.0000000+03	9.19676337+01	9.174730R7+01
4.1000000+03	9.23346R57+01	9.21396500+01
4.2000000+03	9.26929367+01	9.25303173+01
4.3000000+03	9.304279R1+01	9.291R8591+01
4.4000000+03	9.33846529+01	9.33045731+01
4.5000000+03	9.371R85R5+01	9.3686505R+01
4.6000000+03	9.40457492+01	9.40634532+01
4.7000000+03	9.43656377+01	9.44339601+01
4.8000000+03	9.467R8170+01	9.47963205+01
4.9000000+03	9.49R55624+01	9.514R5775+01
5.0000000+03	9.52R61325+01	9.54R85233+01
5.1000000+03	9.55R07706+01	9.58136992+01
5.2000000+03	9.5869705R+01	9.61213957+01
5.3000000+03	9.61531543+01	9.640R6521+01
5.4000000+03	9.64313209+01	9.66722573+01
5.5000000+03	9.67043979+01	9.690R74R7+01



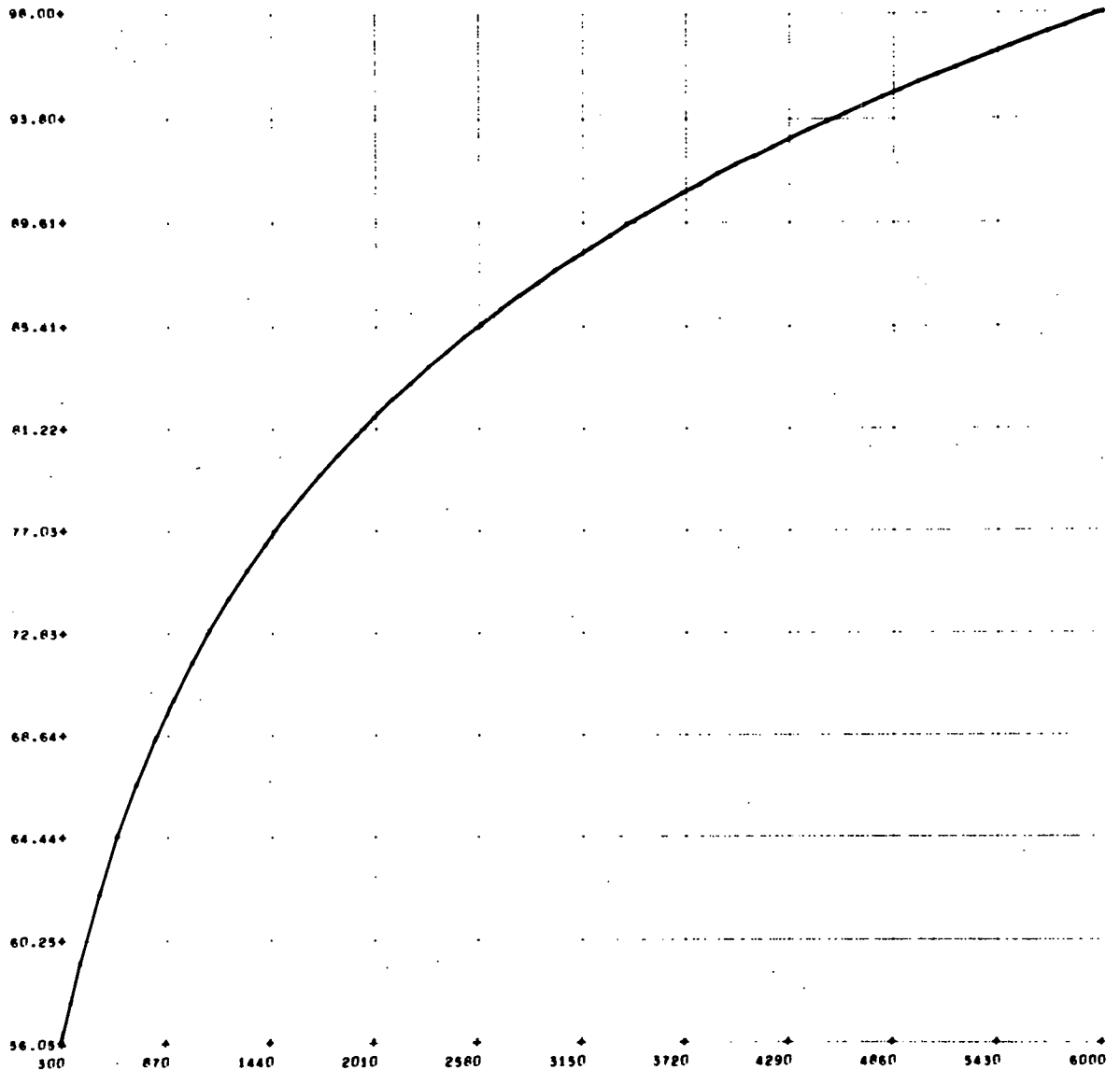
5.60000000+03	9.69725682+01	9.71144133+01
5.70000000+03	9.72360048+01	9.72852869+01
5.80000000+03	9.74948716+01	9.74171543+01
5.90000000+03	9.77493243+01	9.75055504+01
6.00000000+03	9.79995109+01	9.75457575+01





LINEAR POLYATOMIC ALFO
FREE ENERGY (C/M/D) VS TEMPERATURE (DEG K)

CASE THREE



LINEAR POLYATOMIC ALFO CASE THREE
ENTROPY (C/M/D) VS TEMPERATURE (DEG K)

GMX-2 LOADING FORM FOR STRETCH

PROGRAMMER:

PROBLEM: TDF

DATE:

PAGE

OF

±X.XX	±EEE	±X.XX	±EEE	±X.XX	±EEE	±X.XX	±EEE	OF
1	15	19	33	37	51	55	69	73
NON LINEAR POLYATOMIC CF4 CARBON TETRAFLUORIDE CASE FOUR								1
0003								2
+5.801	+001	+1.2	+001					3
+3.	+002	+1.	+002	+6.	+003			4
0001 0000 0004								5
+1.4591	+001	+1.4591	+001	+1.4591	+001			6
+1.	+000							7
+4.345	+002	+2.	+000					8
+6.3	+002	+3.	+000					9
+9.082	+002	+1.	+000					10
+1.277	+003	+3.	+000					11

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NON-LINEAR POLYATOMIC CF4 CARBON TETRAFLUORIDE CASE FOUR

MOLECULAR WT SYMMETRY NO. POLYATOMIC
 8.8100000000+001 1.2000000000+001

 INERTIA A 10+39 INERTIA B 10+39 INERTIA C 10+39 NON-LINEAR
 1.4591000000+001 1.4591000000+001 1.4591000000+001

 G O E
 1.0000000000+000

 VIB FREQ 1/CM DEGENERACY
 4.3480000000+002 2.0000000000+000
 6.3800000000+002 3.0000000000+000
 9.0820000000+002 1.0000000000+000
 1.2770000000+003 3.0000000000+000

FO-HO/T = -4.4561463058E+001 -3.08771779730-002T 8.06415214940-006T+2 -1.18802789487-009T+3 6.84895814996-014T+4

 HO-HO = -3.44312152601+000 1.87817471789-002T 2.85655416351-006T+2 -5.03006344509-010T+3 3.18305926619-014T+4

 SO = 5.13629887515+001 4.59248573880-002T -1.35729300103-005T+2 2.10358403104-009T+3 -1.24349268271-013T+4

TEMP (DEG K)	FO-HO/T (C/M/D)	HO (K/M/D)	SO (C/M/D)	IC
3.0000000+02	-5.23032627+01	3.07235585+00	6.25444489+01	1.23751247+03
4.0000000+02	-5.54503386+01	4.67827529+00	6.71460269+01	1.54402824+03
5.0000000+02	-5.82064703+01	6.51567647+00	7.12378232+01	1.81065003+03
6.0000000+02	-6.06886851+01	8.52357343+00	7.48946408+01	2.01486817+03
7.0000000+02	-6.29567962+01	1.06555708+01	7.81790403+01	2.14557403+03
8.0000000+02	-6.50480628+01	1.28784363+01	8.11461082+01	2.20175179+03
9.0000000+02	-6.69888719+01	1.51687963+01	8.38430901+01	2.18929356+03
1.0000000+03	-6.87993920+01	1.75101655+01	8.63095575+01	2.11814822+03
1.1000000+03	-7.04957367+01	1.98907729+01	8.85782575+01	2.00026695+03
1.2000000+03	-7.20911305+01	2.23020774+01	9.06761951+01	1.84823822+03
1.3000000+03	-7.35966193+01	2.47377752+01	9.26256772+01	1.67441424+03
1.4000000+03	-7.50215457+01	2.71931348+01	9.44452134+01	1.49036571+03
1.5000000+03	-7.63738893+01	2.96645481+01	9.61502547+01	1.30655224+03
1.6000000+03	-7.76605209+01	3.21492229+01	9.77537852+01	1.13213400+03
1.7000000+03	-7.88873972+01	3.46449686+01	9.92667906+01	9.74877095+02
1.8000000+03	-8.00597152+01	3.71300454+01	1.00698629+02	8.41121654+02
1.9000000+03	-8.11820339+01	3.96630549+01	1.02057526+02	7.35792673+02
2.0000000+03	-8.22583732+01	4.21828622+01	1.03349804+02	6.62480350+02
2.1000000+03	-8.32922948+01	4.47085364+01	1.04582074+02	6.23301108+02
2.2000000+03	-8.42869681+01	4.72393080+01	1.05759381+02	6.19373344+02
2.3000000+03	-8.52452248+01	4.97745350+01	1.06886327+02	6.50503766+02
2.4000000+03	-8.61696051+01	5.23136782+01	1.07966971+02	7.15481487+02
2.5000000+03	-8.70623953+01	5.48562814+01	1.09004908+02	8.12137836+02
2.6000000+03	-8.79256605+01	5.74019561+01	1.10003336+02	9.37450455+02
2.7000000+03	-8.87612719+01	5.99503696+01	1.10963112+02	1.08765062+03
2.8000000+03	-8.95709299+01	6.25012352+01	1.11892800+02	1.25833303+03
2.9000000+03	-9.03561844+01	6.50543048+01	1.12788703+02	1.44456753+03
3.0000000+03	-9.11184515+01	6.76093624+01	1.13654908+02	1.64101222+03
3.1000000+03	-9.18590287+01	7.01662193+01	1.14493293+02	1.84202787+03



3.20000000+03	-9.25791073+01	7.27247097+01	1.15305579+02	2.04179309+03
3.30000000+03	-9.32797839+01	7.52846876+01	1.16093326+02	2.23442034+03
3.40000000+03	-9.39620700+01	7.78460238+01	1.16897959+02	2.41407248+03
3.50000000+03	-9.46269006+01	8.04086037+01	1.17600787+02	2.57507979+03
3.60000000+03	-9.52751413+01	8.29723250+01	1.18323009+02	2.71205738+03
3.70000000+03	-9.59075957+01	8.55370963+01	1.19025730+02	2.82002289+03
3.80000000+03	-9.65250102+01	8.81028359+01	1.19709967+02	2.89451450+03
3.90000000+03	-9.71280802+01	9.06694702+01	1.20378662+02	2.9370010+03
4.00000000+03	-9.77174539+01	9.32369327+01	1.21026687+02	2.92954062+03
4.10000000+03	-9.82937369+01	9.58051635+01	1.21660850+02	2.8821858+03
4.20000000+03	-9.88574957+01	9.83741084+01	1.22279902+02	2.79334670+03
4.30000000+03	-9.94092608+01	1.00943718+02	1.22884544+02	2.66004160+03
4.40000000+03	-9.99495300+01	1.03515947+02	1.23475427+02	2.48405167+03
4.50000000+03	-1.00478771+02	1.06084755+02	1.24053161+02	2.26787592+03
4.60000000+03	-1.00997423+02	1.08656105+02	1.24618315+02	2.0158295+03
4.70000000+03	-1.01505900+02	1.11227962+02	1.25171424+02	1.73242994+03
4.80000000+03	-1.02004593+02	1.13800294+02	1.25712987+02	1.42598174+03
4.90000000+03	-1.02493869+02	1.16373073+02	1.26243476+02	1.10522989+03
5.00000000+03	-1.02974077+02	1.18946272+02	1.26763332+02	7.81211806+02
5.10000000+03	-1.03445546+02	1.21519867+02	1.27272971+02	4.67029915+02
5.20000000+03	-1.03908587+02	1.24093835+02	1.27772786+02	1.77970823+02
5.30000000+03	-1.04363496+02	1.26668155+02	1.28263147+02	-6.83754783+01
5.40000000+03	-1.04810552+02	1.29242807+02	1.28744405+02	-2.51996388+02
5.50000000+03	-1.05250021+02	1.31817774+02	1.29216889+02	-3.5037466+02
5.60000000+03	-1.05682156+02	1.34393038+02	1.29680913+02	-3.38183175+02
5.70000000+03	-1.06107197+02	1.36968585+02	1.30136774+02	-1.87537623+02
5.80000000+03	-1.06525374+02	1.39544399+02	1.30584753+02	1.32494715+02
5.90000000+03	-1.06936902+02	1.42120467+02	1.31025117+02	6.55828284+02
6.00000000+03	-1.07341991+02	1.44696777+02	1.31458120+02	1.41951574+03
6.10000000+03	-1.07740888+02	1.47273317+02	1.31884004+02	2.46386726+03
6.20000000+03	-1.08133632+02	1.49850075+02	1.32302998+02	3.83256983+03
6.30000000+03	-1.08520553+02	1.52427041+02	1.32715322+02	5.57280661+03

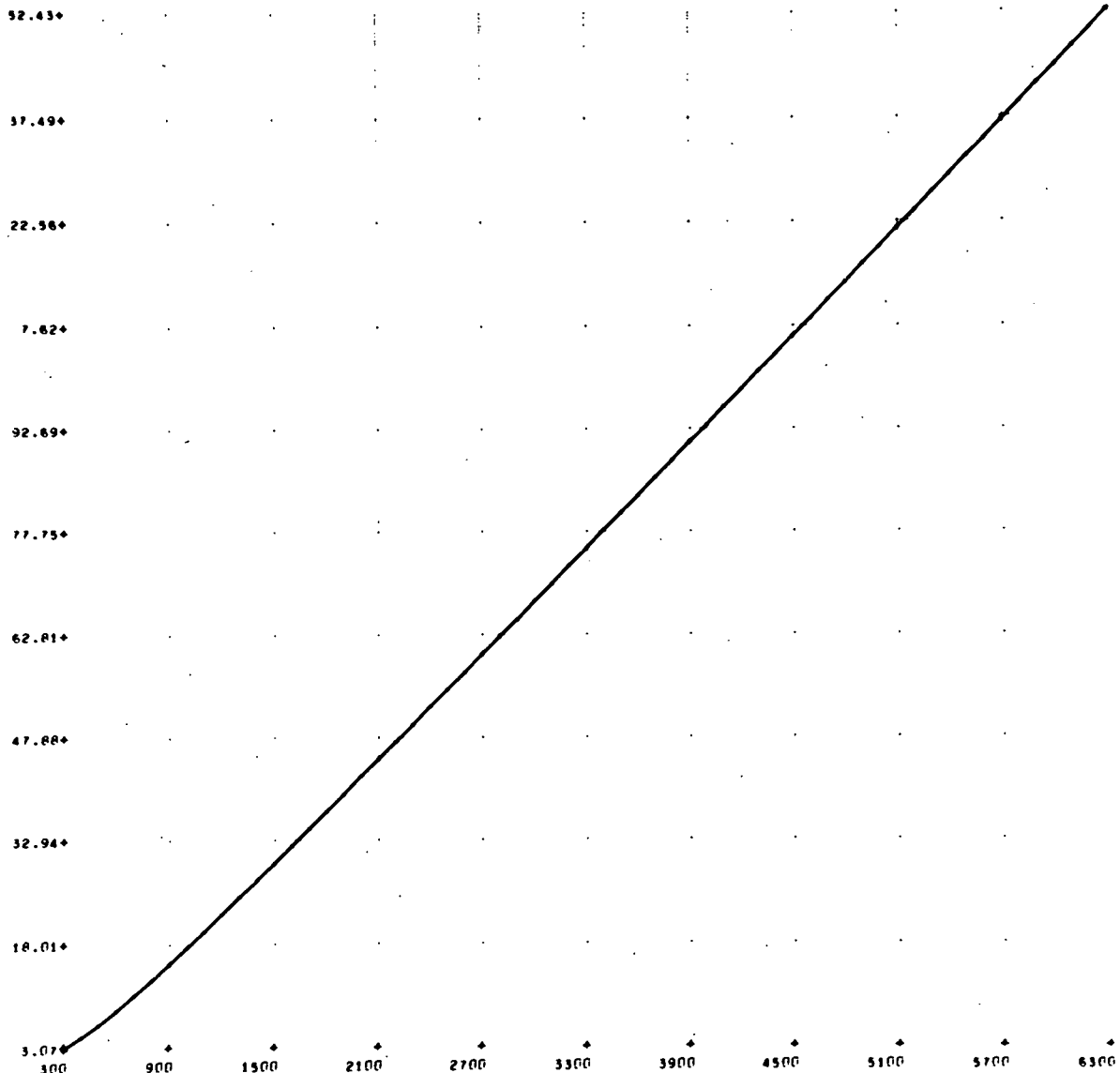
ENTROPY FIT

VARIANCE
1.52171297145-001

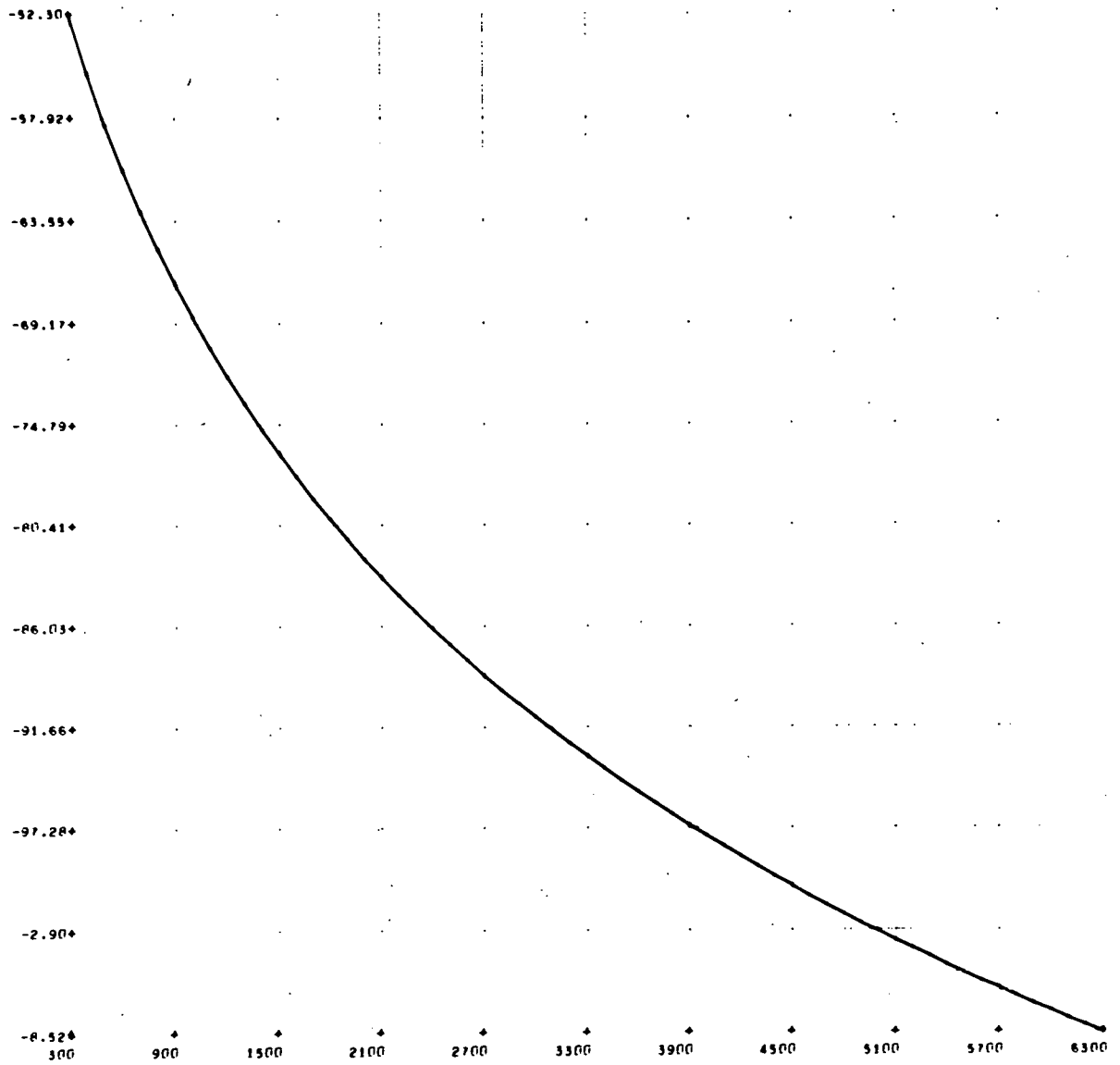
TEMP (DEG K)	SG	SG FROM FIT
3.0000000+02	6.25444489+01	6.39746418+01
4.0000000+02	6.71460269+01	6.76926789+01
5.0000000+02	7.12378232+01	7.11873311+01
6.0000000+02	7.48946408+01	7.44698769+01
7.0000000+02	7.81790403+01	7.75512963+01
8.0000000+02	8.11461082+01	8.04422710+01
9.0000000+02	8.38430901+01	8.31531843+01
1.0000000+03	8.63095575+01	8.56941209+01
1.1000000+03	8.85782575+01	8.80748671+01
1.2000000+03	9.06761951+01	9.03049110+01
1.3000000+03	9.26256772+01	9.23934418+01
1.4000000+03	9.44452134+01	9.43493507+01
1.5000000+03	9.61502547+01	9.61812302+01
1.6000000+03	9.77537852+01	9.78973746+01
1.7000000+03	9.92667906+01	9.95057794+01
1.8000000+03	1.00698629+02	1.01014142+02
1.9000000+03	1.02057326+02	1.02429861+02
2.0000000+03	1.03349804+02	1.03760037+02
2.1000000+03	1.04582074+02	1.05011473+02
2.2000000+03	1.05759381+02	1.06190670+02
2.3000000+03	1.06886327+02	1.07303836+02
2.4000000+03	1.07966971+02	1.08356875+02
2.5000000+03	1.09004908+02	1.09355397+02
2.6000000+03	1.10003336+02	1.10304711+02
2.7000000+03	1.10965112+02	1.11209828+02
2.8000000+03	1.11892800+02	1.12075462+02
2.9000000+03	1.12788703+02	1.12906027+02
3.0000000+03	1.13654906+02	1.13705639+02
3.1000000+03	1.14495293+02	1.14478115+02
3.2000000+03	1.15305579+02	1.15226975+02
3.3000000+03	1.16093326+02	1.15955439+02
3.4000000+03	1.16857959+02	1.16666429+02
3.5000000+03	1.17600787+02	1.17362370+02
3.6000000+03	1.18323009+02	1.18046187+02
3.7000000+03	1.19023730+02	1.18719306+02
3.8000000+03	1.19709967+02	1.19383657+02
3.9000000+03	1.20376662+02	1.20040669+02
4.0000000+03	1.21026687+02	1.20691473+02
4.1000000+03	1.21660850+02	1.21336904+02
4.2000000+03	1.22279902+02	1.21977496+02
4.3000000+03	1.22884544+02	1.22613485+02
4.4000000+03	1.23475427+02	1.23244809+02
4.5000000+03	1.24053161+02	1.23871107+02
4.6000000+03	1.24618315+02	1.24491721+02
4.7000000+03	1.25171424+02	1.25105693+02
4.8000000+03	1.25712987+02	1.25711767+02
4.9000000+03	1.26243476+02	1.26308389+02
5.0000000+03	1.26763332+02	1.26893707+02
5.1000000+03	1.27272971+02	1.27465568+02
5.2000000+03	1.27772786+02	1.28021523+02
5.3000000+03	1.28263147+02	1.28558825+02
5.4000000+03	1.28744405+02	1.29074426+02
5.5000000+03	1.29216889+02	1.29564982+02



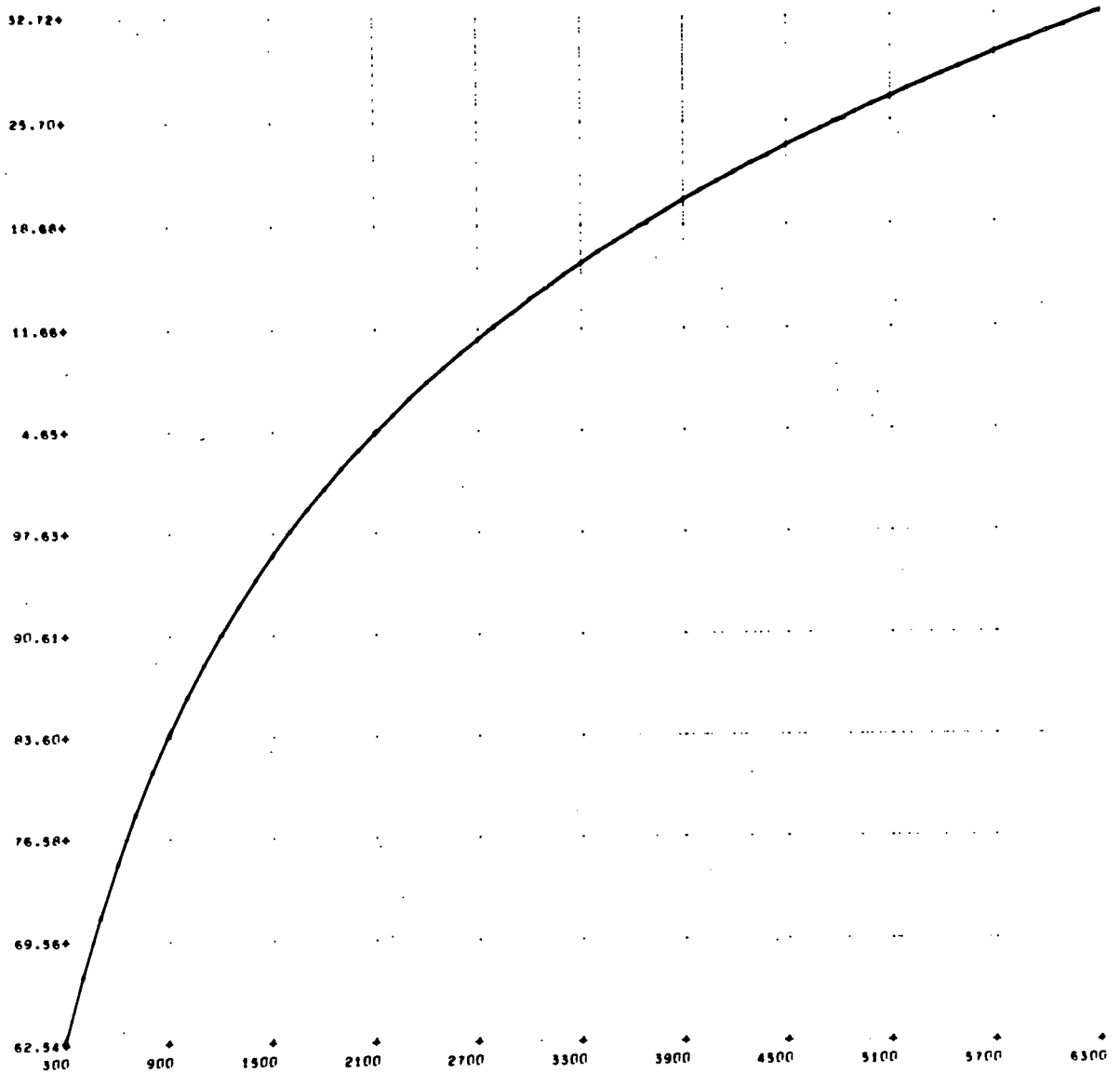
5.6000000+03	1.29600913+02	1.30026850+02
5.7000000+03	1.30136774+02	1.30456087+02
5.8000000+03	1.30584753+02	1.30884854+02
5.9000000+03	1.31025117+02	1.31199411+02
6.0000000+03	1.31458120+02	1.31504122+02
6.1000000+03	1.31884004+02	1.31757450+02
6.2000000+03	1.32302998+02	1.31953963+02
6.3000000+03	1.32715322+02	1.32087927+02



NON LINEAR POLYATOMIC CF4 CARBON TETRAFLUORIDE CASE FOUR
 ENTHALPY (KCAL/M) VS TEMPERATURE (DEG K)



NON LINEAR POLYATOMIC CF4 CARBON TETRAFLUORIDE CASE FOUR
FREE ENERGY (C/M/D) VS TEMPERATURE (DEG K)



NON LINEAR POLYATOMIC CF4 CARBON TETRAFLUORIDE CASE FOUR
ENTROPY (C/M/D) VS TEMPERATURE (DEG K)

GMX-2 LOADING FORM FOR STRETCH

PROGRAMMER:

PROBLEM: TDF

DATE:

PAGE

OF

±X.XX	±EEE	±X.XX	±EEE	±X.XX	±EEE	±X.XX	±EEE	Card no.
1	5	19	33	37	51	55	69	73
POLYATOMIC WITH MOMENT OF INERTIA COMPUTED LIZO CASE FIVE								1
C.C.C.3								2
+2.988	+0.01	+2.	+0.00					3
+3.	+0.02	+1.	+0.02	+6.	+0.03			4
C.C.C.1 C.C.C.3 C.C.C.3								5
+6.94	+0.00	-1.667	+0.00	+1.277	+0.00	+0.	+0.00	6
+1.6	+0.01	+0.	+0.00	+0.	+0.00	+0.	+0.00	7
+6.94	+0.00	+1.667	+0.00	+1.277	+0.00	+0.	+0.00	8
+1.	+0.00							9
+1.27	+0.03	+1.	+0.00					10
+7.4	+0.02	+1.	+0.00					11
+1.65	+0.03	+1.	+0.00					12

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POLYATOMIC WITH MOMENT OF INERTIA COMPUTED L120 CASE FIVE

MOLECULAR WT 2.9880000000+001 SYMMETRY NO. 2.0000000000+000 POLYATOMIC

INERTIA A 10*59 2.01238140962+000 INERTIA B 10*59 6.40413255140+000 INERTIA C 10*59 8.41651396102+000 NON-LINEAR

CO E 1.0000000000+000

VIB FREQ 1/CM DEGENERACY

1.2700000000+003 1.0000000000+000

7.4000000000+002 1.0000000000+000

1.6500000000+003 1.0000000000+000

FO-HO/T = -4.37285298795+001 -2.07475486776-002T 6.30371786460-006T*2 -1.03247438552-009T*3 6.46848983760-014T*4

H-HO = -8.65792933211-001 9.81373121211-003T 1.66662210926-006T*2 -2.99960546100-010T*3 1.95804613590-014T*4

SO = 5.06278443597+001 2.53405665693-002T -7.80964080719-006T*2 1.26820910184-009T*3 -7.86653794072-014T*4

TEMP (DEG K)	FO-HO/T (C/M/D)	HO (KC/M)	SO (C/M/D)	IC
3.0000000+02	-4.85090074+01	2.45720190+00	5.66996804+01	1.44989850+03
4.0000000+02	-5.09023236+01	3.38887987+00	5.93745233+01	1.67114070+03
5.0000000+02	-5.28271461+01	4.39756763+00	6.16222814+01	1.82331954+03
6.0000000+02	-5.44598774+01	5.47459367+00	6.35842002+01	1.91950366+03
7.0000000+02	-5.58903551+01	6.60800295+00	6.53303593+01	1.96757295+03
8.0000000+02	-5.71702992+01	7.78644113+00	6.69033506+01	1.97417838+03
9.0000000+02	-5.83323832+01	9.00045950+00	6.83328938+01	1.94612238+03
1.0000000+03	-5.93987888+01	1.02426122+01	6.96414010+01	1.89033158+03
1.1000000+03	-6.03854377+01	1.15071532+01	7.08464860+01	1.81462941+03
1.2000000+03	-6.13042615+01	1.27896700+01	7.19623198+01	1.72544520+03
1.3000000+03	-6.21645065+01	1.40867637+01	7.30004786+01	1.62956977+03
1.4000000+03	-6.29735292+01	1.53957976+01	7.39705275+01	1.53297961+03
1.5000000+03	-6.37373073+01	1.67147081+01	7.48804460+01	1.44092323+03
1.6000000+03	-6.44607817+01	1.80418642+01	7.57369468+01	1.35785647+03
1.7000000+03	-6.51480943+01	1.93759647+01	7.65457207+01	1.28741468+03
1.8000000+03	-6.58027592+01	2.07159613+01	7.73116266+01	1.23241170+03
1.9000000+03	-6.64277877+01	2.20610017+01	7.80388412+01	1.19485847+03
2.0000000+03	-6.70257830+01	2.34103869+01	7.87309765+01	1.17599586+03
2.1000000+03	-6.75990132+01	2.47635391+01	7.93911747+01	1.17633793+03
2.2000000+03	-6.81494675+01	2.61199770+01	8.00221843+01	1.19572276+03
2.3000000+03	-6.86789011+01	2.74792966+01	8.06264214+01	1.23336899+03
2.4000000+03	-6.91888715+01	2.88411567+01	8.12060202+01	1.28793664+03
2.5000000+03	-6.96807675+01	3.02052672+01	8.17628744+01	1.35759102+03
2.6000000+03	-7.01558326+01	3.15713802+01	8.22986712+01	1.44006918+03
2.7000000+03	-7.06151857+01	3.29392824+01	8.28149199+01	1.53274810+03
2.8000000+03	-7.10598366+01	3.43087894+01	8.33129757+01	1.63271445+03
2.9000000+03	-7.14907003+01	3.56797413+01	8.37940594+01	1.73683536+03
3.0000000+03	-7.19086885+01	3.70519984+01	8.42592747+01	1.84185014+03
3.1000000+03	-7.23143195+01	3.84254383+01	8.47096222+01	1.94434265+03
3.2000000+03	-7.2708265+01	3.97999535+01	8.51460120+01	2.04101424+03

3.50000000+03	-7.30910052+01	4.11751400+01	8.53692740+01	2.12055710+03
3.40000000+03	-7.34064919+01	4.25510402+01	8.59001870+01	2.20902035+03
3.50000000+03	-7.38282203+01	4.39290320+01	8.63793064+01	2.28390331+03
3.60000000+03	-7.41622000+01	4.53070192+01	8.67673712+01	2.30615053+03
3.70000000+03	-7.45273503+01	4.66930003+01	8.71653097+01	2.32830591+03
3.80000000+03	-7.48664655+01	4.80649020+01	8.75131450+01	2.32056730+03
3.90000000+03	-7.51934053+01	4.94440762+01	8.78173709+01	2.30590965+03
4.00000000+03	-7.55147467+01	5.08253193+01	8.82210765+01	2.28665906+03
4.10000000+03	-7.58200323+01	5.22062718+01	8.85620695+01	2.18776060+03
4.20000000+03	-7.61359035+01	5.35876377+01	8.89090991+01	2.09359207+03
4.30000000+03	-7.64364994+01	5.49695064+01	8.92201191+01	1.97764526+03
4.40000000+03	-7.67306610+01	5.63510434+01	8.95370901+01	1.84233203+03
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4.80000000+03	-7.78487962+01	6.18845653+01	9.07414140+01	1.19008306+03
4.90000000+03	-7.81148327+01	6.32685390+01	9.10267794+01	1.03119022+03
5.00000000+03	-7.83750775+01	6.46529200+01	9.13064359+01	8.89542472+02
5.10000000+03	-7.86321146+01	6.60373003+01	9.15800064+01	7.76642063+02
5.20000000+03	-7.88857179+01	6.74220720+01	9.18495011+01	7.04737644+02
5.30000000+03	-7.91309520+01	6.88070710+01	9.21133103+01	6.47607634+02
5.40000000+03	-7.93736729+01	7.01922923+01	9.23722453+01	7.40035691+02
5.50000000+03	-7.96123206+01	7.15777222+01	9.26264599+01	8.81406111+02
5.60000000+03	-7.98469936+01	7.29633506+01	9.28761294+01	1.12095792+03
5.70000000+03	-8.00776995+01	7.43491671+01	9.31214130+01	1.50298707+03
5.80000000+03	-8.03046751+01	7.57351620+01	9.33624016+01	2.02744040+03
5.90000000+03	-8.05280073+01	7.71213263+01	9.35994105+01	2.72604450+03
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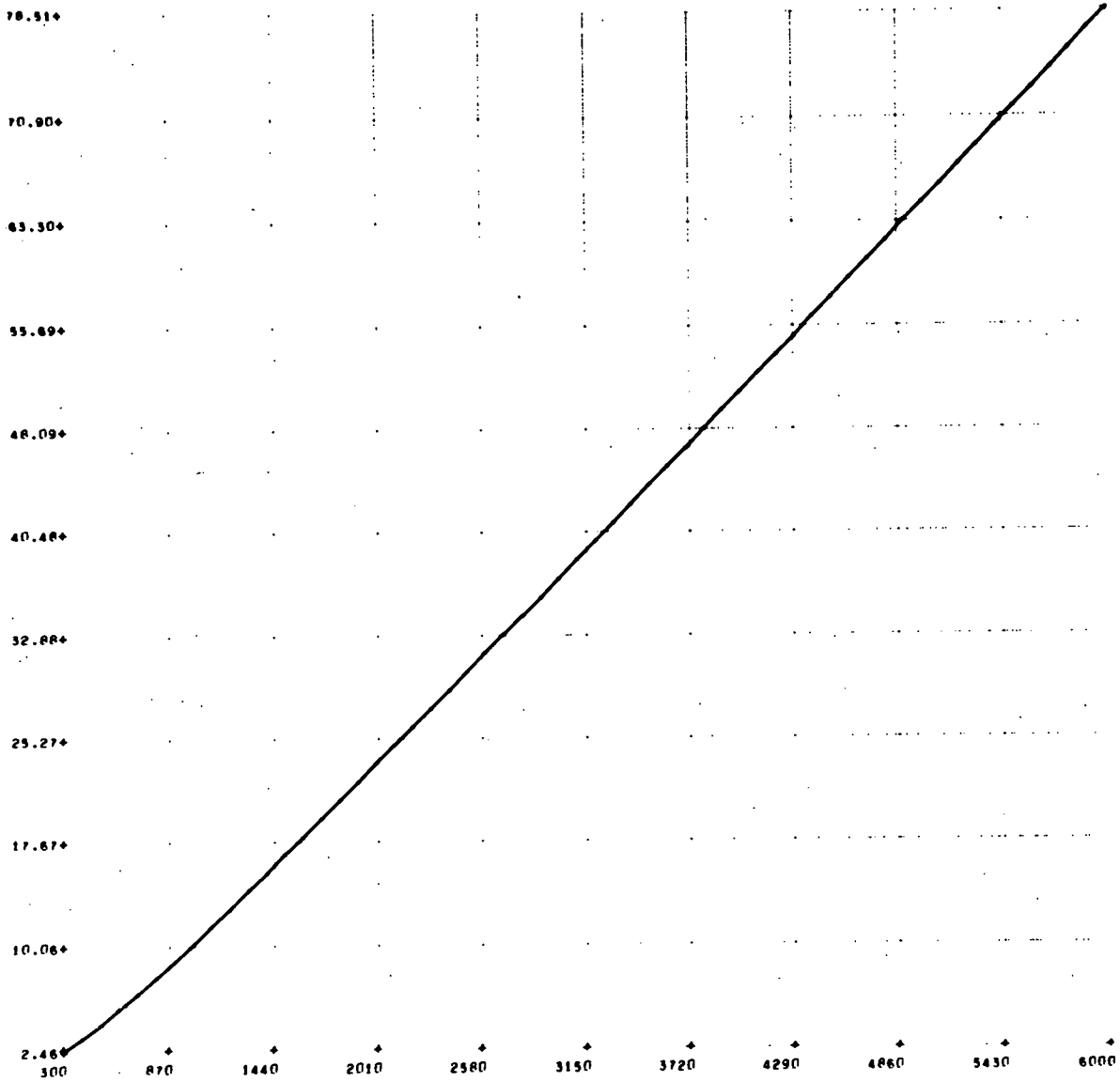
ENTROPY FIT

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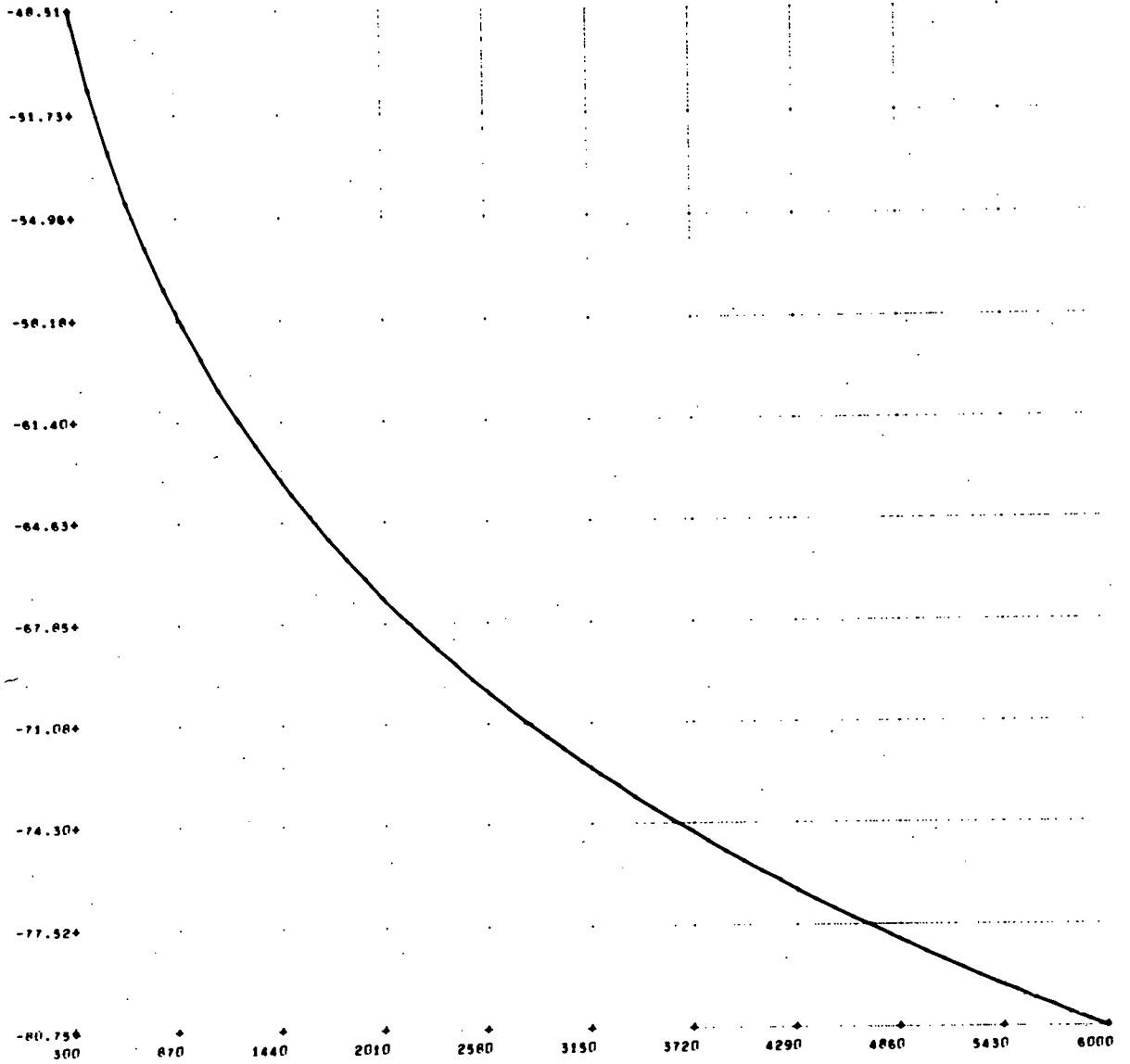
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4.0000000+02	5.93745233+01	5.95936800+01
5.0000000+02	6.16222814+01	6.14993270+01
6.0000000+02	6.35842002+01	6.32844517+01
7.0000000+02	6.53303593+01	6.49556251+01
8.0000000+02	6.69033506+01	6.65192292+01
9.0000000+02	6.83328938+01	6.79814573+01
1.0000000+03	6.96414010+01	6.93483138+01
1.1000000+03	7.08464860+01	7.06256145+01
1.2000000+03	7.19623198+01	7.18189863+01
1.3000000+03	7.30004786+01	7.29338671+01
1.4000000+03	7.39705273+01	7.39755064+01
1.5000000+03	7.48804460+01	7.49489646+01
1.6000000+03	7.57369468+01	7.58591135+01
1.7000000+03	7.65457207+01	7.67106358+01
1.8000000+03	7.73116266+01	7.75080258+01
1.9000000+03	7.80388412+01	7.82555887+01
2.0000000+03	7.87309765+01	7.89574410+01
2.1000000+03	7.93911747+01	7.96175105+01
2.2000000+03	8.00221843+01	8.02395361+01
2.3000000+03	8.06264214+01	8.08270679+01
2.4000000+03	8.12060202+01	8.13834672+01
2.5000000+03	8.17628744+01	8.19119066+01
2.6000000+03	8.22986712+01	8.24153697+01
2.7000000+03	8.28149199+01	8.28966516+01
2.8000000+03	8.33129757+01	8.33583583+01
2.9000000+03	8.37940594+01	8.38029072+01
3.0000000+03	8.42592747+01	8.42325268+01
3.1000000+03	8.47096222+01	8.46492569+01
3.2000000+03	8.51460120+01	8.50549485+01
3.3000000+03	8.55692740+01	8.54512636+01
3.4000000+03	8.59801670+01	8.58396757+01
3.5000000+03	8.63793864+01	8.62214692+01
3.6000000+03	8.67675712+01	8.65977400+01
3.7000000+03	8.71453097+01	8.69693950+01
3.8000000+03	8.75131450+01	8.73371524+01
3.9000000+03	8.78715789+01	8.77015416+01
4.0000000+03	8.82210765+01	8.80629031+01
4.1000000+03	8.85620695+01	8.84213887+01
4.2000000+03	8.88949591+01	8.87769614+01
4.3000000+03	8.92201191+01	8.91293954+01
4.4000000+03	8.95378981+01	8.94782760+01
4.5000000+03	8.98486219+01	8.98229998+01
4.6000000+03	9.01525930+01	9.01627747+01
4.7000000+03	9.04501031+01	9.04966197+01
4.8000000+03	9.07414140+01	9.08233688+01
4.9000000+03	9.10267794+01	9.11416516+01
5.0000000+03	9.13064359+01	9.14499326+01
5.1000000+03	9.15806064+01	9.17484717+01
5.2000000+03	9.18495011+01	9.20293438+01
5.3000000+03	9.21133183+01	9.22964352+01
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5.5000000+03	9.26264599+01	9.27738766+01



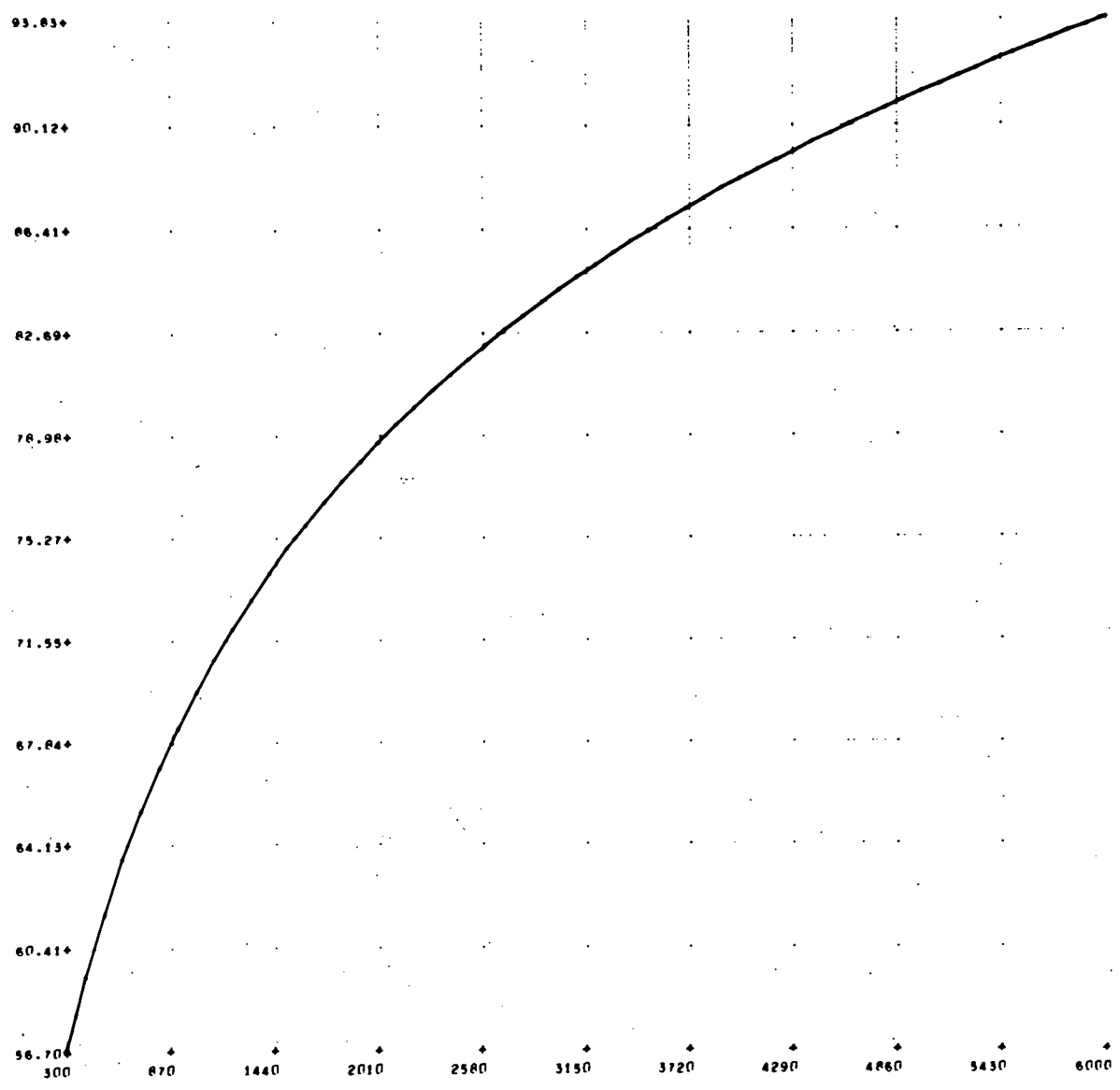
5.60000000+03	9.28761294+01	9.29790552+01
5.70000000+03	9.31214130+01	9.31581098+01
5.80000000+03	9.33624616+01	9.33079828+01
5.90000000+03	9.35994185+01	9.34254277+01
6.00000000+03	9.38324198+01	9.35070090+01



POLYATOMIC WITH MOMENT OF INERTIA COMPUTED LI2O CASE FIVE
 ENTHALPY (KJ/M) VS TEMPERATURE (DEG K)



POLYATOMIC WITH MOMENT OF INERTIA COMPUTED L120 CASE FIVE
 FREE ENERGY(H/D) VS TEMPERATURE (DEG K)



POLYATOMIC WITH MOMENT OF INERTIA COMPUTED L120 CASE FIVE
ENTROPY (C/M/D) VS TEMPERATURE (DEG K)

GMX-2 LOADING FORM FOR STRETCH

PROGRAMMER:

PROBLEM: TDF

DATE:

PAGE

OF

±X.XX	±EEE	±X.XX	±EEE	±X.XX	±EEE	±X.XX	±EEE	Card no.
	15	19	33	37	51	55	69	73
ONE DEBYE THETA SOLID B BORDON						CASE SIX		1
GCCY								2
+1.25	+0.03							3
+1.	+0.00	+3.	+0.00					4
+3.	+0.02	+1.	+0.02	+6.	+0.03			5

-52-

ONE DEBYE THETA SOLID B BORON

CASE SIX

DEBYE TEMP DIMENSION NUMBER OF ATOMS/CELL
 1.2400000000+003 3.0000000000+000 1.0000000000+000

FO-HQ/T = 1.1419299R131+000 -5.34763R142RR-003T 1.0956RRR759-006T*2 -1.35270345R92-010T*3 6.8R92RRR4R40-015T*4

H-HQ = -1.2169947R424+000 4.2R76R671625-003T 7.26460362596-007T*2 -1.35R1R2R915-010T*3 9.0R5R59R127-015T*4

SG = -1.52461R3132R+000 1.0R527371135-002T -3.30055121950-006T*2 5.29400511539-010T*3 -5.251723R15R1-014T*4

CV = 2.31490720239+000 4.9517371R065-003T -2.3464R559462-006T*2 4.5R006063153-010T*3 -3.1415777R17R-014T*4

TEMP (CEG K)	FO-HQ/T (C/M/D)	HQ (KC/M)	SG (C/M/D)	CV (C/M/D)	IC
3.00000000+02	-4.2R697161-01	3.019912R3-01	1.43533477+00	2.85301476+00	-1.3012R60+02
4.00000000+02	-R.00R41564-01	6.39575R59-01	2.3997R121+00	3.8272R4R7+00	-9.77176995+01
5.00000000+02	-1.21434694+00	1.0556033R+00	3.3255370+00	4.44645466+00	-4.99455417+01
6.00000000+02	-1.63R05R16+00	1.52155533+00	4.1739R372+00	4.8444R742+00	-6.092R7145+00
7.00000000+02	-2.05611355+00	2.0201093R+00	4.9419R409+00	5.10955340+00	2.49551734+01
8.00000000+02	-2.46099437+00	2.54076251+00	5.63694751+00	5.292R242R+00	4.05671457+01
9.00000000+02	-2.84950059+00	3.07694RR6+00	6.26R33266+00	5.4239515R+00	4.05143511+01
1.00000000+03	-3.22064127+00	3.6244111R+00	6.84505245+00	5.52061310+00	2.73735135+01
1.10000000+03	-3.57454265+00	4.1R029069+00	7.374R0691+00	5.59372412+00	3.647R5216+00
1.20000000+03	-3.911R7790+00	4.74260609+00	7.86404964+00	5.6502609R+00	-2.7726676+01
1.30000000+03	-4.23556622+00	5.30994544+00	8.31R13964+00	5.694R2666+00	-6.3R3R2R61+01
1.40000000+03	-4.54061341+00	5.8R12775R+00	8.74152597+00	5.73054641+00	-1.0199676R+02
1.50000000+03	-4.83402R07+00	6.455R3310+00	9.137916R0+00	5.75959705+00	5.75959705+00
1.60000000+03	-5.11477902+00	7.033026R6+00	9.510420R1+00	5.78352972+00	-1.751064R2+02
1.70000000+03	-5.3R377524+00	7.61240636+00	9.86166134+00	5.80347234+00	-2.06239225+02
1.80000000+03	-5.641R5R10+00	8.19361639+00	1.0193R672+01	5.82026021+00	-2.31R02435+02
1.90000000+03	-5.8R9R0037+00	8.77637436+00	1.050R944R+01	5.83452205+00	-2.5076R6R0+02
2.00000000+03	-6.12R30R37+00	9.36045273+00	1.0R0R5351+01	5.84673R12+00	-2.62446501+02
2.10000000+03	-6.35R02R13+00	9.9456662R+00	1.10940597+01	5.8572R022+00	-2.66461916+02
2.20000000+03	-6.57954639+00	1.0531R62R+01	1.13667567+01	5.8664396R+00	-2.62736574+02
2.30000000+03	-6.79339962+00	1.111R9159+01	1.16277109+01	5.87444732+00	-2.51463526+02
2.40000000+03	-7.0000769R+00	1.17067200+01	1.1R77R770+01	5.8R14R790+00	-2.330R1309+02
2.50000000+03	-7.2000252R+00	1.22951R62+01	1.211R099R+01	5.8R771063+00	-2.0R246772+02
2.60000000+03	-7.39365322+00	1.2R42390+01	1.23491297+01	5.89323713+00	-1.77R00006+02
2.70000000+03	-7.5R133523+00	1.3473R13R+01	1.25716366+01	5.89R16727+00	-1.42770575+02
2.80000000+03	-7.763414R+00	1.4063R553+01	1.27862203+01	5.9025R367+00	-1.0427R245+02
2.90000000+03	-7.94020797+00	1.46543157+01	1.29934203+01	5.90655515+00	-6.35733045+01
3.00000000+03	-R.11200529+00	1.52451534+01	1.31937231+01	5.91013942+00	-2.19715966+01
3.10000000+03	-R.27907502+00	1.5R363323+01	1.33R75693+01	5.9133R513+00	1.91R6R9R5+01
3.20000000+03	-R.44166496+00	1.6427R206+01	1.357335R9+01	5.91633353+00	5.84774592+01
3.30000000+03	-R.6000443+00	1.70195903+01	1.37574560+01	5.919019R1+00	9.46031691+01
3.40000000+03	-R.75430601+00	1.7611616R+01	1.39341933+01	5.92147409+00	1.26243577+02
3.50000000+03	-R.9047670R+00	1.8203R7R2+01	1.4105R752+01	5.92372230+00	1.52176452+02
3.60000000+03	-9.05157119+00	1.87963551+01	1.42727R10+01	5.9257R6R5+00	1.71290419+02
3.70000000+03	-9.194R9929+00	1.93R90301+01	1.44351677+01	5.9276R71R+00	1.82615R4R+02
3.80000000+03	-9.334R8R82+00	1.99R1R77+01	1.45932723+01	5.92944024+00	1.85355R02+02
3.90000000+03	-9.47169472+00	2.0574913R+01	1.47473136+01	5.931060R4+00	1.7R21017+02
4.00000000+03	-9.60547029+00	2.116R0959+01	1.4R974943+01	5.932619R+00	1.62940935+02
4.10000000+03	-9.73633R01+00	2.17614226+01	1.50440021+01	5.93395513+00	1.37334719+02
4.20000000+03	-9.86442024+00	2.2354R36+01	1.51R70116+01	5.93525037+00	1.023023R0+02
4.30000000+03	-9.9R9R31R6+00	2.294R4697+01	1.53266R53+01	5.93645666+00	5.8375R195+01



4.40000000+03	-1.01126809+01	2.35421723+01	1.54631746+01	5.93758196+00	6.44596057+00
4.50000000+03	-1.02330690+01	2.41359836+01	1.55966209+01	5.93863335+00	-5.22061296+01
4.60000000+03	-1.03510920+01	2.47298967+01	1.57271565+01	5.93961716+00	-1.15878110+02
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4.80000000+03	-1.05803990+01	2.59180026+01	1.59799828+01	5.94140412+00	-2.49179100+02
4.90000000+03	-1.06918490+01	2.65121841+01	1.61024988+01	5.94221693+00	-3.15016685+02
5.00000000+03	-1.08012666+01	2.71064444+01	1.62225554+01	5.94298160+00	-3.70228980+02
5.10000000+03	-1.09087240+01	2.77007789+01	1.63402493+01	5.94370186+00	-4.16539915+02
5.20000000+03	-1.10142898+01	2.82951854+01	1.64556712+01	5.94438009+00	-4.47065156+02
5.30000000+03	-1.11180290+01	2.88896538+01	1.65689071+01	5.94502233+00	-4.56280926+02
5.40000000+03	-1.12200034+01	2.94841867+01	1.66800379+01	5.94562837+00	-4.47992819+02
5.50000000+03	-1.13202716+01	3.00787784+01	1.67891404+01	5.94620174+00	-3.85304605+02
5.60000000+03	-1.14188895+01	3.06734260+01	1.68962870+01	5.94674474+00	-2.90870040+02
5.70000000+03	-1.15159102+01	3.12681264+01	1.70015464+01	5.94725948+00	-1.45446673+02
5.80000000+03	-1.16113844+01	3.18628770+01	1.71049839+01	5.94774788+00	5.03053565+01
5.90000000+03	-1.17053604+01	3.24576752+01	1.72066613+01	5.94821171+00	3.33684516+02
6.00000000+03	-1.17978842+01	3.30525186+01	1.73066373+01	5.94865259+00	6.88564882+02

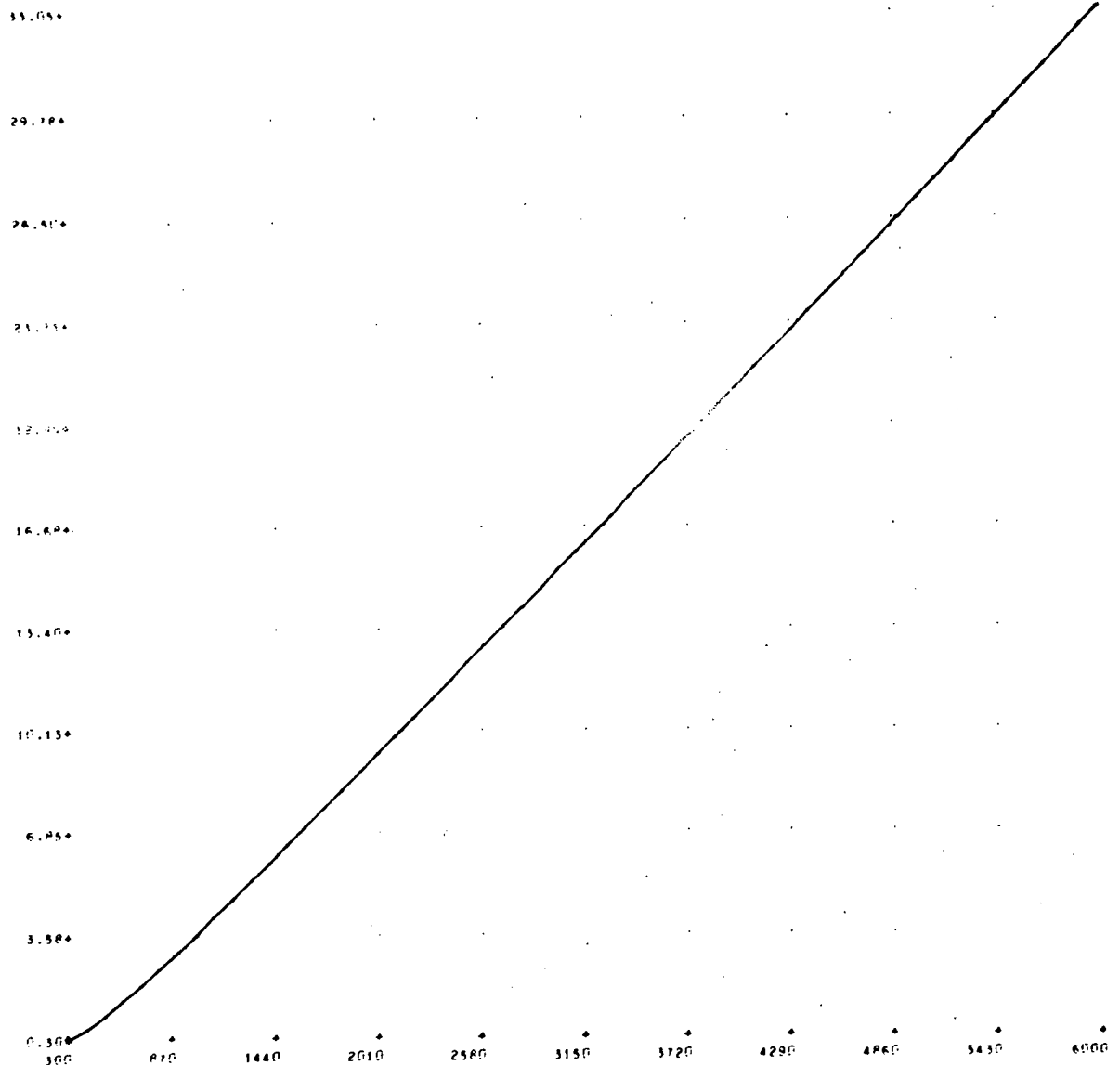
ENTROPY FIT

VARIANCE
5.50409940242-003

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6.00000000+02	4.17398372+00	4.10896179+00
7.00000000+02	4.94198409+00	4.82880456+00
8.00000000+02	5.63694751+00	5.50295260+00
9.00000000+02	6.26833266+00	6.13399701+00
1.00000000+03	6.84505245+00	6.72445085+00
1.10000000+03	7.37480691+00	7.27674913+00
1.20000000+03	7.86404964+00	7.79324881+00
1.30000000+03	8.31813964+00	8.27622881+00
1.40000000+03	8.74152597+00	8.72789004+00
1.50000000+03	9.13791680+00	9.15035532+00
1.60000000+03	9.51042081+00	9.54566947+00
1.70000000+03	9.86166134+00	9.91579924+00
1.80000000+03	1.01938672+01	1.02626334+01
1.90000000+03	1.05089448+01	1.05879825+01
2.00000000+03	1.08083351+01	1.08935793+01
2.10000000+03	1.10940597+01	1.11810784+01
2.20000000+03	1.13667567+01	1.14520563+01
2.30000000+03	1.16277109+01	1.17080115+01
2.40000000+03	1.18778770+01	1.19503645+01
2.50000000+03	1.21180998+01	1.21804577+01
2.60000000+03	1.23491297+01	1.23995556+01
2.70000000+03	1.25716366+01	1.26088444+01
2.80000000+03	1.27862203+01	1.28094325+01
2.90000000+03	1.29934203+01	1.30023502+01
3.00000000+03	1.31937231+01	1.31885496+01
3.10000000+03	1.33875693+01	1.33689049+01
3.20000000+03	1.35753589+01	1.35442124+01
3.30000000+03	1.37574560+01	1.37151900+01
3.40000000+03	1.39341933+01	1.38824779+01
3.50000000+03	1.41058752+01	1.40466380+01
3.60000000+03	1.42727810+01	1.42081544+01
3.70000000+03	1.44351677+01	1.43674330+01
3.80000000+03	1.45932723+01	1.45248016+01
3.90000000+03	1.47473136+01	1.46805101+01
4.00000000+03	1.48974943+01	1.48347304+01
4.10000000+03	1.50440021+01	1.49875562+01
4.20000000+03	1.51870116+01	1.51390032+01
4.30000000+03	1.53266853+01	1.52890091+01
4.40000000+03	1.54631746+01	1.54374335+01
4.50000000+03	1.55966209+01	1.55840581+01
4.60000000+03	1.57271565+01	1.57285865+01
4.70000000+03	1.58549051+01	1.58706441+01
4.80000000+03	1.59799828+01	1.60097784+01
4.90000000+03	1.61024988+01	1.61454588+01
5.00000000+03	1.62225554+01	1.62770769+01
5.10000000+03	1.63402493+01	1.64039458+01
5.20000000+03	1.64556712+01	1.65253009+01
5.30000000+03	1.65689871+01	1.66402996+01
5.40000000+03	1.66800379+01	1.67480210+01
5.50000000+03	1.67891404+01	1.68474663+01

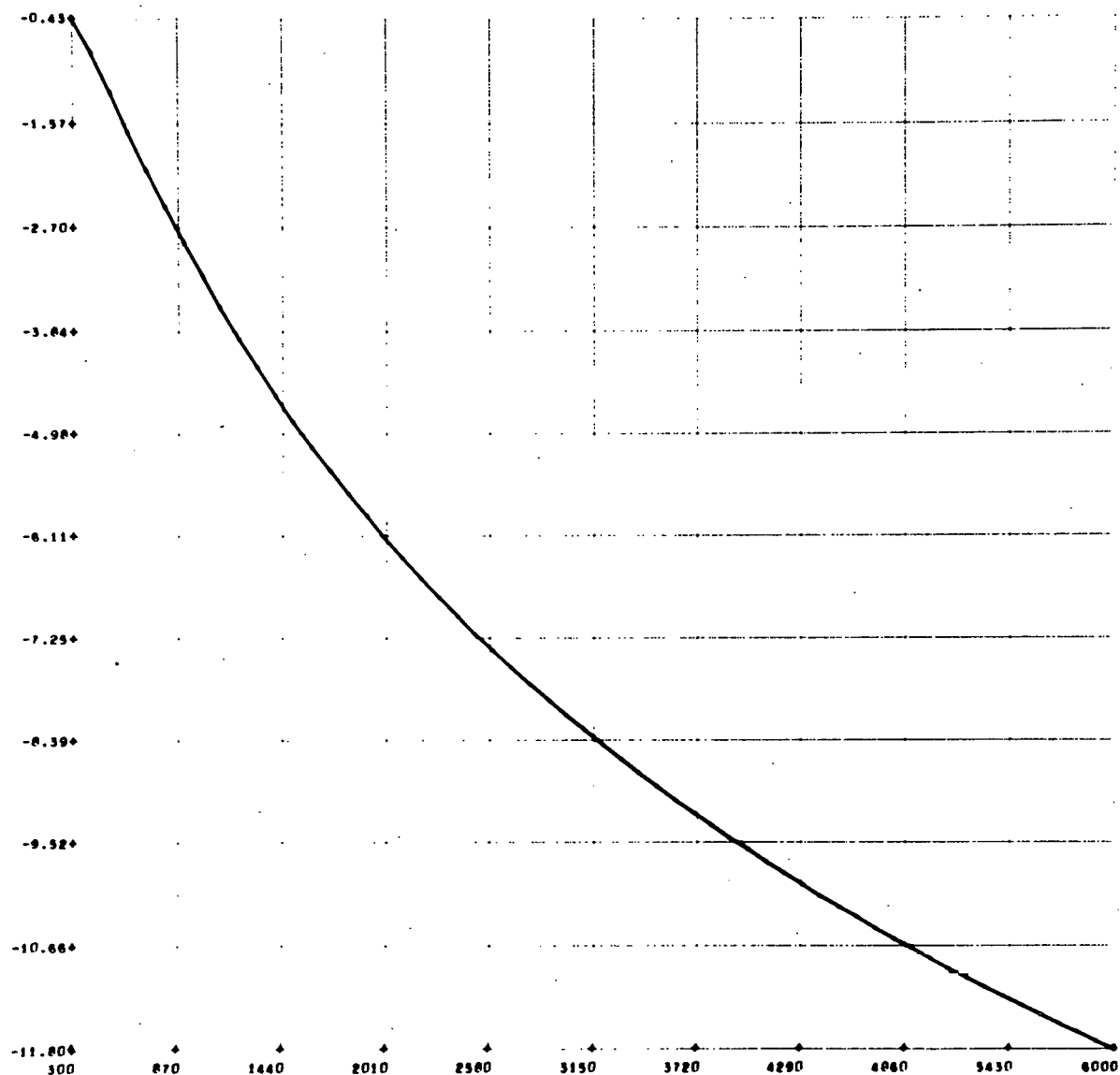


5.4000000+03	1.6896287+01	1.6937558+01
5.7000000+03	1.70015464+01	1.70171452+01
5.8000000+03	1.71049839+01	1.70849870+01
5.9000000+03	1.72066613+01	1.71397790+01
6.0000000+03	1.73064373+01	1.71801303+01



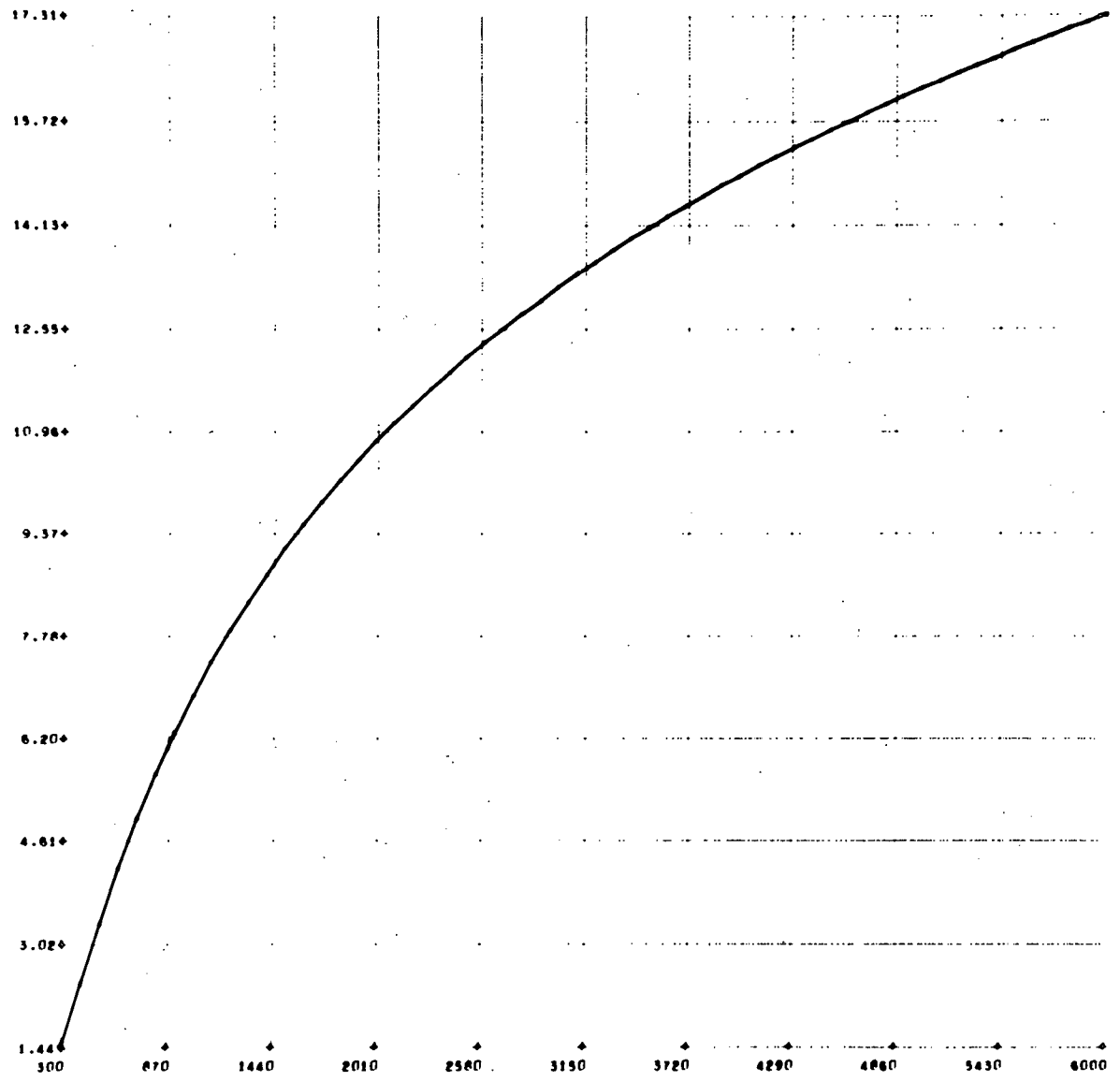
ONE DEBYE META SOLID B BORON
ENTHALPY (KJ/M) VS TEMPERATURE (DEG K)

CASE SIX



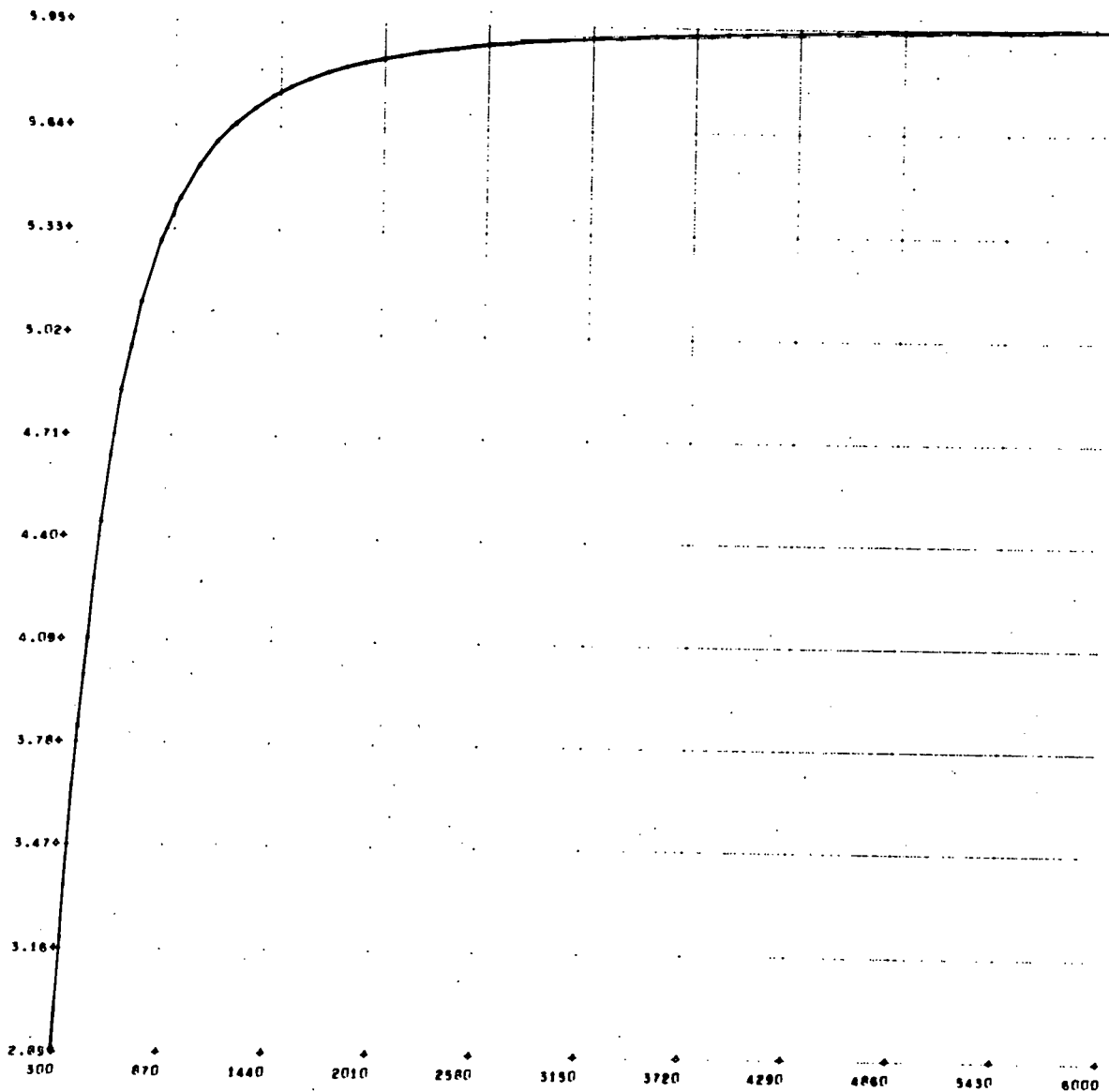
ONE DEBYE META SOLID B BORON
FREE ENERGY (C/M/D) VS TEMPERATURE (DEG K)

CASE SIX



ONE DEBYE THETA SOLID B BORON
ENTROPY (C/M/D) VS TEMPERATURE (DEG K)

CASE SIX



ONE DEBYE THETA SOLID B BORON CASE SIX
 HEAT CAPACITY (C/M/O) VS TEMPERATURE (DEG K)



GMX-2 LOADING FORM FOR STRETCH

PROGRAMMER:

PROBLEM: TDF

DATE:

PAGE

OF

±X.XX	±EEE	±X.XX	±EEE	±X.XX	±EEE	±X.XX	±EEE	OF
1	15	19	33	37	51	55	69	73
TUG DEBYE THETA	SOLID	BM	BORN	MIRIDE		CASE	SEVEN	1
G.C.C.5								2
+8.5	+0.02	+2.1	+0.03					3
+2.	+0.00							4
+3.	+0.02	+1.	+0.02	+6.	+0.03			5

-61-

TWO CEBYTE META SOLID BN BORON NITRIDE CASE SEVEN

CEBYE TEMP (TRAN)	CEBYE TEMP (LONG)	DIMENSION	NUMBER OF ATOMS/CELL
8.500000000+002	2.100000000+003	2.000000000+000	2.000000000+000
FG-H0/T = 1.55101693511+000	-9.89012342950-003T	1.96340524142-006T02	-2.4011534645-010T03 1.22734213267-014T04
H-H0 = -2.05081407906+000	7.30404468644-003T	1.94042176891-006T02	-3.55974748409-010T03 2.3526618211-014T04
SO = -1.57042757728+000	1.95900021233-002T	-5.64193175049-006T02	8.76696310502-010T03 -5.27755261909-014T04
CV = 3.37380825260+000	1.09106940813-002T	-4.99552040105-006T02	9.54718474987-010T03 -6.45715614564-014T04

TEMP (DEG R)	FG-H0/T (C/M/D)	H0 (KC/M)	SO (C/M/D)	CV (C/M/D)	IC
3.0000000+002	-1.35168046+000	6.62100006-01	3.55870715+00	5.11209733+00	-1.23110653+02
4.0000000+002	-2.11599941+000	1.29494401+00	5.25335944+00	6.68082763+00	-8.79339696+01
5.0000000+002	-2.90764837+000	1.98580210+00	6.87925256+00	7.87797016+00	-5.25629419+01
6.0000000+002	-3.69774175+000	2.82010695+00	8.39791999+00	8.76265624+00	2.44129143+01
7.0000000+002	-4.47072835+000	3.73053434+00	9.80006311+00	9.41288460+00	7.03045398+01
8.0000000+002	-5.21864085+000	4.69710032+00	1.10900163+01	9.89499411+00	9.85926926+01
9.0000000+002	-5.93788126+000	5.70557206+00	1.22774058+01	1.02577798+01	1.07130433+02
1.0000000+003	-6.62734017+000	6.74582784+00	1.33731680+01	1.05353645+01	9.68127997+01
1.1000000+003	-7.28729537+000	7.81059840+00	1.43878394+01	1.07313159+01	7.02393350+01
1.2000000+003	-7.91876932+000	8.89458674+00	1.53309249+01	1.09219795+01	3.09104033+01
1.3000000+003	-8.52315571+000	9.99387059+00	1.62107485+01	1.10588235+01	-1.73196163+01
1.4000000+003	-9.10200359+000	1.11054987+01	1.70345027+01	1.11700114+01	-7.05954119+01
1.5000000+003	-9.65689405+000	1.22272161+01	1.78083715+01	1.12614453+01	-1.25284809+02
1.6000000+003	-1.01893715+001	1.33572749+01	1.85376683+01	1.13374579+01	-1.78117519+02
1.7000000+003	-1.07009072+001	1.44943021+01	1.92269672+01	1.14012773+01	-2.26265650+02
1.8000000+003	-1.11928816+001	1.56372059+01	1.98802182+01	1.14553421+01	-2.67388751+02
1.9000000+003	-1.16665783+001	1.67851081+01	2.05008458+01	1.15015189+01	-2.99648567+02
2.0000000+003	-1.21231842+001	1.79372953+01	2.10918318+01	1.15412536+01	-3.21708568+02
2.1000000+003	-1.25637926+001	1.90931821+01	2.16557841+01	1.15756790+01	-3.32719467+02
2.2000000+003	-1.29894094+001	2.02522842+01	2.21949931+01	1.16056917+01	-3.32295809+02
2.3000000+003	-1.34009591+001	2.14141974+01	2.27114797+01	1.16320087+01	-3.20889396+02
2.4000000+003	-1.37992913+001	2.25785821+01	2.32070338+01	1.16552081+01	-2.97737251+02
2.5000000+003	-1.41851873+001	2.37451509+01	2.36832476+01	1.16757600+01	-2.64857614+02
2.6000000+003	-1.45593660+001	2.49136588+01	2.41415424+01	1.16940498+01	-2.22974456+02
2.7000000+003	-1.49224896+001	2.60838961+01	2.45831919+01	1.17103958+01	-1.73491580+02
2.8000000+003	-1.52751690+001	2.72556820+01	2.50093412+01	1.17250623+01	-1.18044529+02
2.9000000+003	-1.56179683+001	2.84288600+01	2.54210235+01	1.17382707+01	-5.84547550+01
3.0000000+003	-1.59514090+001	2.96032938+01	2.58191736+01	1.17502069+01	3.31713411+00
3.1000000+003	-1.62759742+001	3.07788642+01	2.62046401+01	1.17610286+01	6.52189621+01
3.2000000+003	-1.65921119+001	3.19554668+01	2.65781953+01	1.17708697+01	1.25154849+02
3.3000000+003	-1.690022381+001	3.31330093+01	2.69403439+01	1.17798448+01	1.81033934+02
3.4000000+003	-1.72007397+001	3.43114102+01	2.72923309+01	1.17880520+01	2.30819168+02
3.5000000+003	-1.74939770+001	3.54905970+01	2.76341476+01	1.17955764+01	2.72576512+02
3.6000000+003	-1.77802862+001	3.66705052+01	2.79665376+01	1.18024913+01	3.04524366+02
3.7000000+003	-1.80599810+001	3.78510771+01	2.82900018+01	1.18088606+01	3.25083187+02
3.8000000+003	-1.83335549+001	3.90322610+01	2.86050025+01	1.18147400+01	3.32925271+02
3.9000000+003	-1.86008626+001	4.02140104+01	2.89119673+01	1.18201784+01	3.17024669+02
4.0000000+003	-1.88622218+001	4.13962834+01	2.92112927+01	1.18252187+01	3.06070705+02
4.1000000+003	-1.91182143+001	4.25790421+01	2.95033465+01	1.18298988+01	2.71700599+02
4.2000000+003	-1.93688871+001	4.37622523+01	2.97874709+01	1.18342519+01	2.22184655+02
4.3000000+003	-1.96144540+001	4.49458826+01	3.00669849+01	1.18383080+01	1.58841520+02



4.40000000+03	-1.98551164+01	4.61299048+01	3.05391857+01	1.18420932+01	8.29059950+01
4.50000000+03	-2.00910641+01	4.73142930+01	3.06053514+01	1.18456312+01	-3.78410532+00
4.60000000+03	-2.03224761+01	4.84990235+01	3.06657421+01	1.18489429+01	-9.87375574+01
4.70000000+03	-2.05495218+01	4.96840747+01	3.11206015+01	1.18520473+01	-1.98759297+02
4.80000000+03	-2.07723612+01	5.08694266+01	3.13701584+01	1.18549612+01	-2.98999959+02
4.90000000+03	-2.09911458+01	5.20550611+01	3.16146277+01	1.18576999+01	-3.97405392+02
5.00000000+03	-2.12060193+01	5.32409612+01	3.18542115+01	1.18602771+01	-4.95666159+02
5.10000000+03	-2.14171177+01	5.44271116+01	3.20891004+01	1.18627053+01	-5.93167000+02
5.20000000+03	-2.16245704+01	5.56134977+01	3.23194738+01	1.18649957+01	-6.90743630+02
5.30000000+03	-2.18285000+01	5.68001065+01	3.25455012+01	1.18671585+01	-6.24995566+02
5.40000000+03	-2.20290234+01	5.79869255+01	3.27673430+01	1.18692031+01	-6.01308776+02
5.50000000+03	-2.22262517+01	5.91739434+01	3.29851505+01	1.18711378+01	-5.25731893+02
5.60000000+03	-2.24202905+01	6.03611496+01	3.31990673+01	1.18729703+01	-3.86462233+02
5.70000000+03	-2.26112408+01	6.15485343+01	3.34092293+01	1.18747079+01	-1.70487880+02
5.80000000+03	-2.27991986+01	6.27360883+01	3.36157656+01	1.18763568+01	1.36462915+02
5.90000000+03	-2.29842558+01	6.39238029+01	3.38187986+01	1.18779230+01	5.49972345+02
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ENTROPY FIT

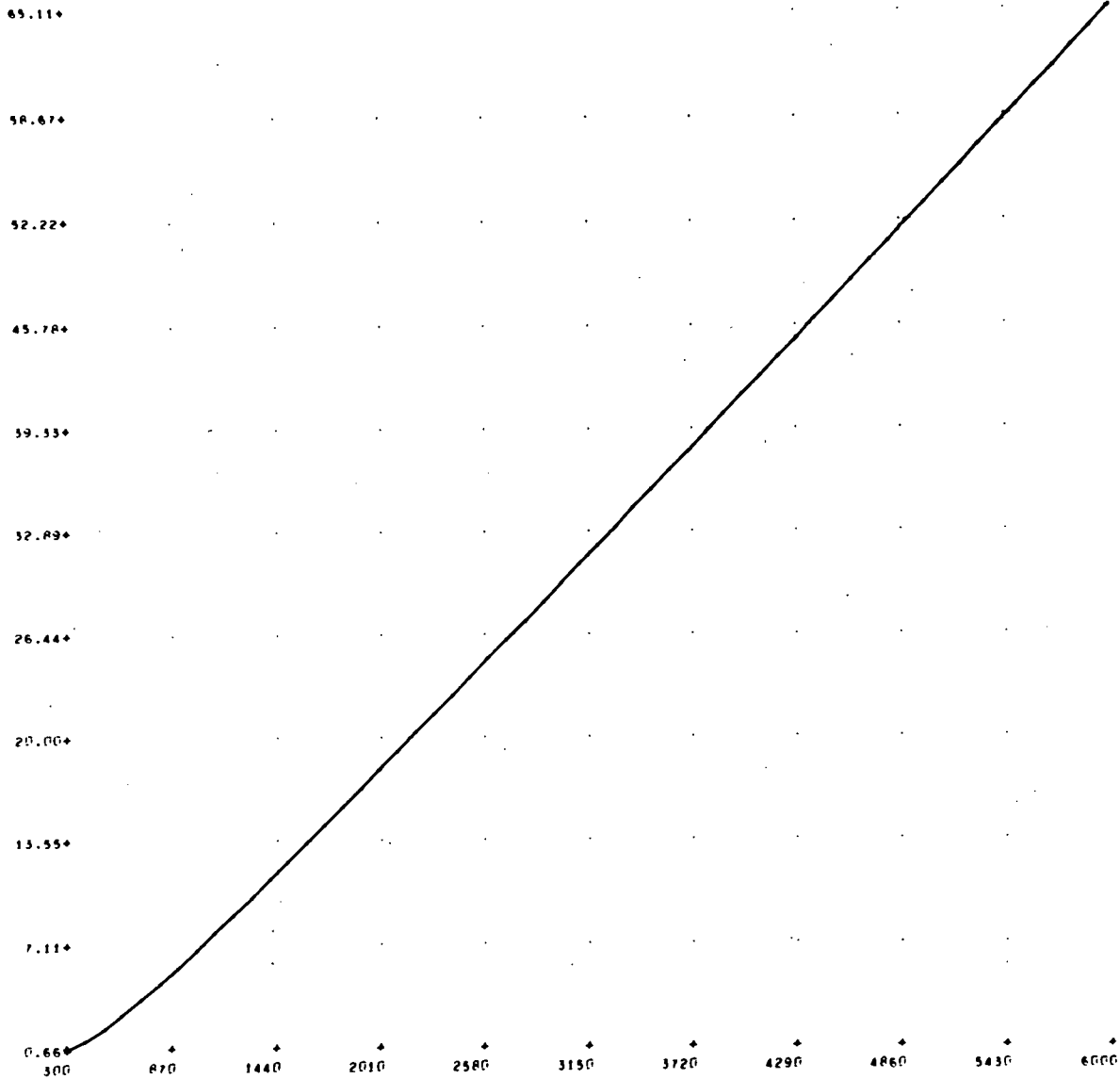
VARIANCE

1.07116941047-002

TEMP (DEG K)	SG	SG FROM FIT
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5.00000000+02	6.87925256+00	6.92037912+00
6.00000000+02	8.39791999+00	8.33500496+00
7.00000000+02	9.80006311+00	9.66606278+00
8.00000000+02	1.10900163+01	1.09179895+01
9.00000000+02	1.22774058+01	1.20950952+01
1.00000000+03	1.33731680+01	1.32015636+01
1.10000000+03	1.43878394+01	1.42414515+01
1.20000000+03	1.53309249+01	1.52186891+01
1.30000000+03	1.62107485+01	1.61370801+01
1.40000000+03	1.70345027+01	1.70003014+01
1.50000000+03	1.78083715+01	1.78119031+01
1.60000000+03	1.85376683+01	1.85753089+01
1.70000000+03	1.92269672+01	1.92938158+01
1.80000000+03	1.98802182+01	1.99705939+01
1.90000000+03	2.05008458+01	2.06086869+01
2.00000000+03	2.10918318+01	2.12110117+01
2.10000000+03	2.16557841+01	2.17803587+01
2.20000000+03	2.21949931+01	2.23193914+01
2.30000000+03	2.27114797+01	2.28306468+01
2.40000000+03	2.32070358+01	2.33165351+01
2.50000000+03	2.36832476+01	2.37793402+01
2.60000000+03	2.41415424+01	2.42212188+01
2.70000000+03	2.45831919+01	2.46442013+01
2.80000000+03	2.50093412+01	2.50501915+01
2.90000000+03	2.54210235+01	2.54409662+01
3.00000000+03	2.58191736+01	2.58181758+01
3.10000000+03	2.62046401+01	2.61833440+01
3.20000000+03	2.65781953+01	2.65378678+01
3.30000000+03	2.69405439+01	2.68830175+01
3.40000000+03	2.72923309+01	2.72199368+01
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4.30000000+03	3.00669849+01	3.00078549+01
4.40000000+03	3.03391857+01	3.02975077+01
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5.20000000+03	3.23194738+01	3.24228256+01
5.30000000+03	3.25455012+01	3.26522088+01
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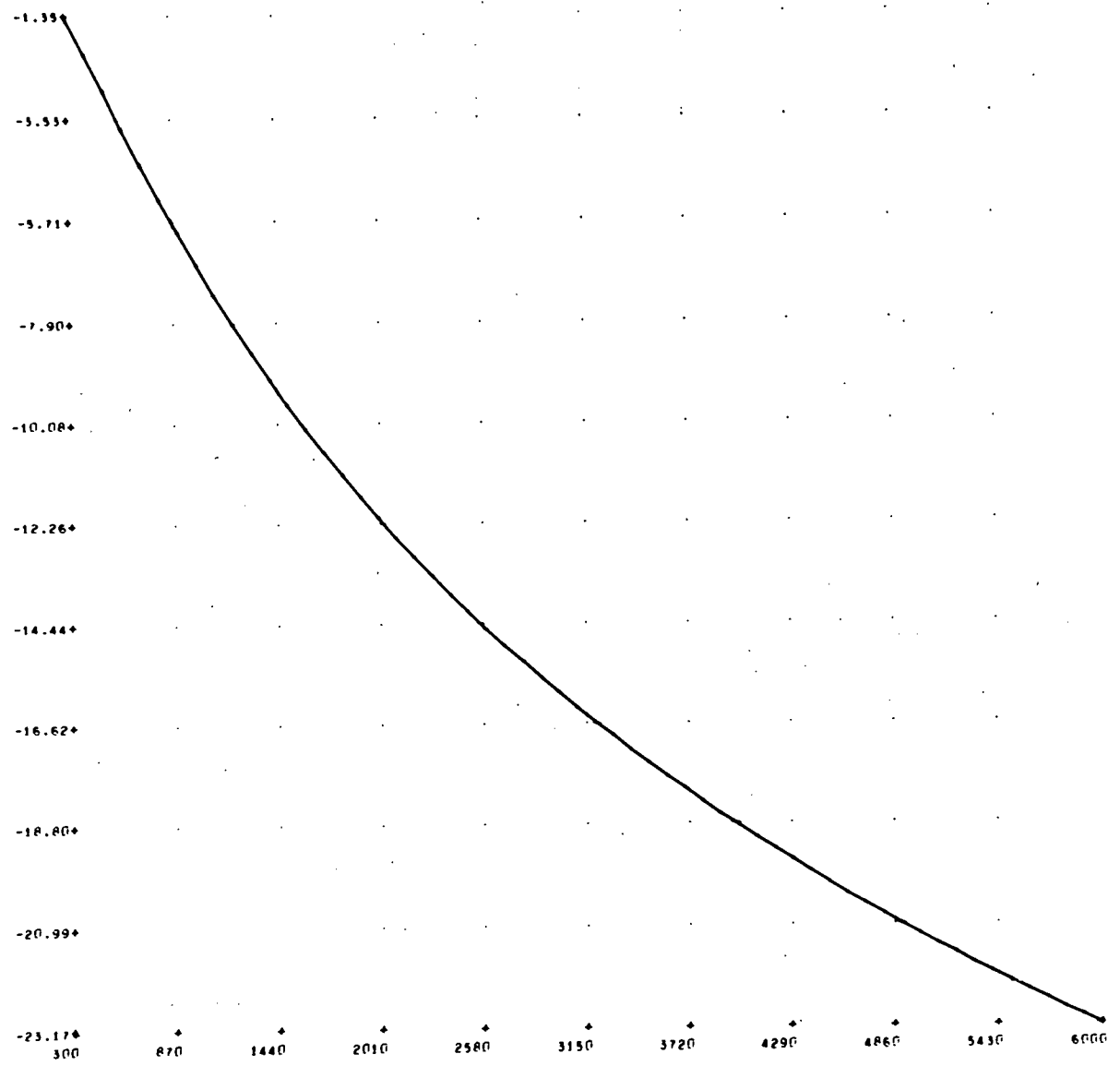


5.60000000+03	5.31990673+01	3.32624338+01
5.70000000+03	5.34092293+01	3.34343911+01
5.80000000+03	5.36197636+01	3.35875681+01
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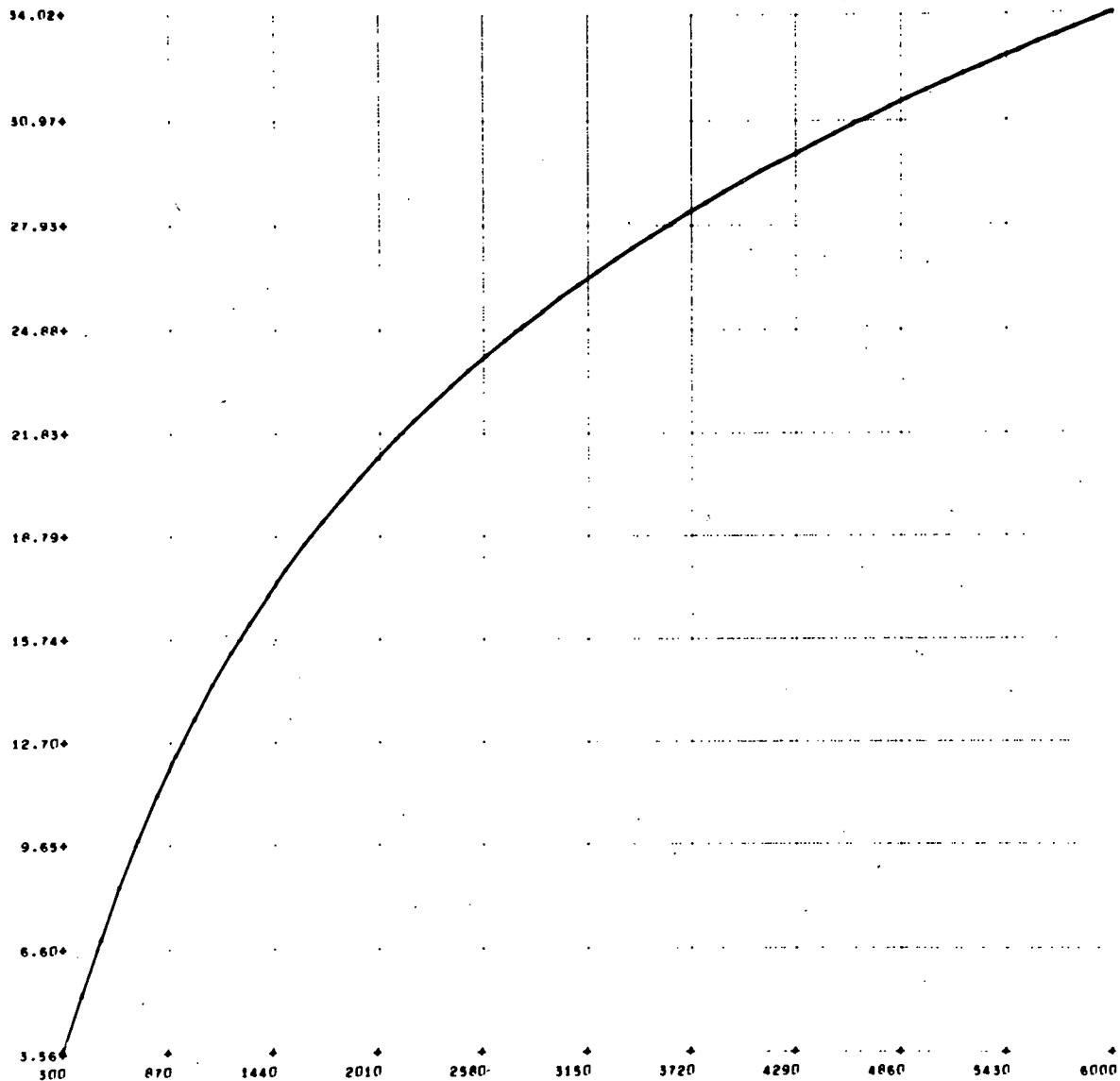


TWO DEBYE THETA SOLID BN BORON NITRIDE
 ENTHALPY (KJ/M) VS TEMPERATURE (DEG K)

CASE SEVEN

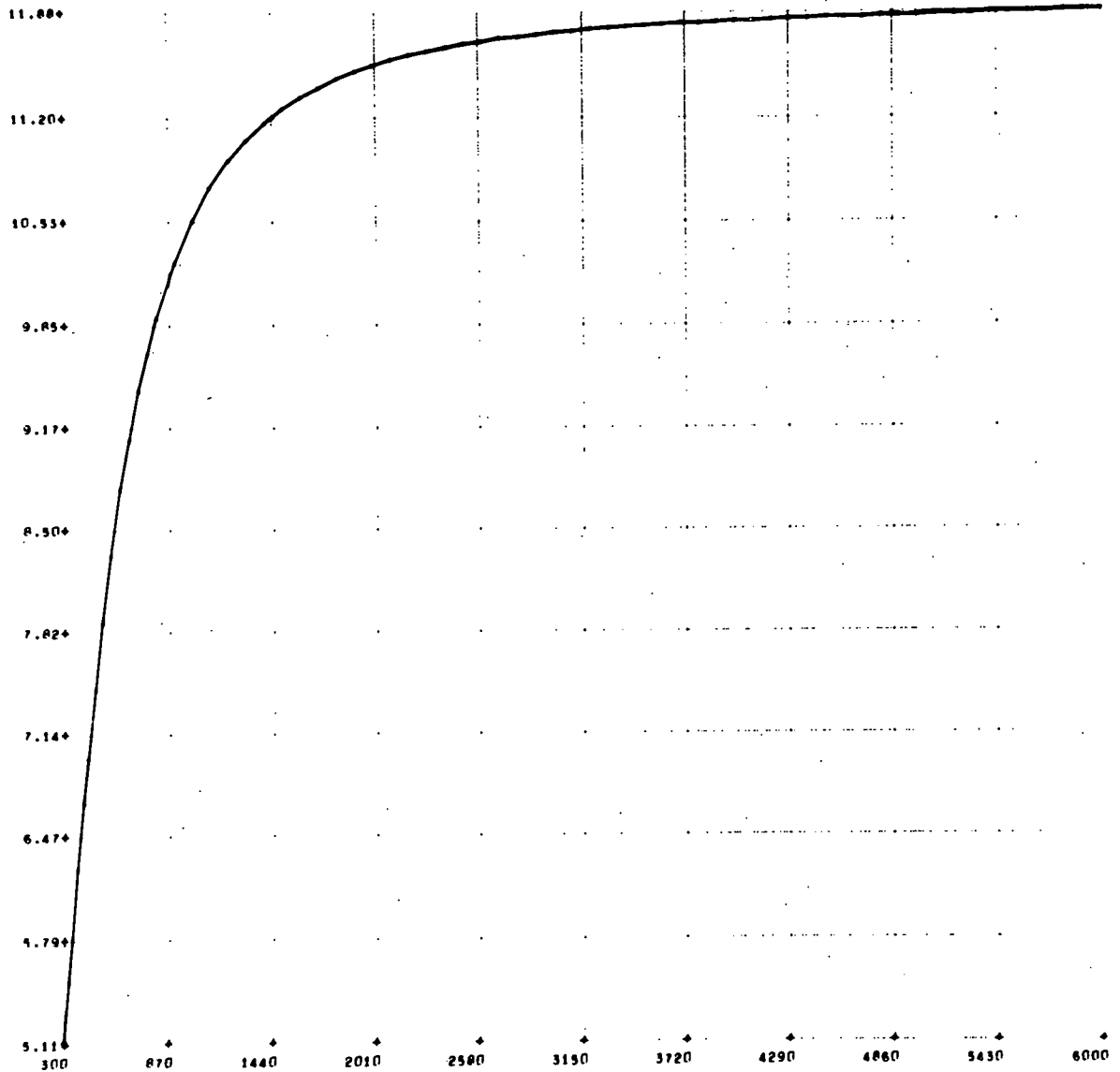


TWO DEBYE THETA SOLID BN BORON NITRIDE CASE SEVEN
FREE ENERGY (C/M/D) VS TEMPERATURE (DEG K)



TWO DEBYE THETA SOLID BN BORON NITRIDE
ENTROPY (C/M/D) VS TEMPERATURE (DEG K)

CASE SEVEN



TWO DEBYE META SOLID BN BORON NITRIDE CASE SEVEN
 HEAT CAPACITY (C/M/D) VS TEMPERATURE (DEG K)

Appendix

MONOATOMIC GAS

The theory of the calculation is described by Rossini⁴.

Translation contribution

$$\frac{F_t}{T} = -(3/2)R \ln M_w - (5/2)R \ln T + 7.28295$$

$$\frac{H_t}{T} = (5/2)R$$

Electronic contribution

$$U_i = \frac{hcT_i}{kT}$$

$$Q_e = g_0 + \sum_i g_i e^{-U_i}$$

$$\frac{F_e}{T} = -R \ln Q_e$$

$$\frac{H_e}{T} = \frac{R}{Q_e} \left(\sum_i U_i g_i e^{-U_i} \right)$$

$$\frac{F^{\circ} - H^{\circ}_0}{T} = \frac{F_t}{T} + \frac{F_e}{T}$$

$$H^{\circ} - H^{\circ}_0 = H_t + H_e$$

DIATOMIC GAS

The method of calculation is that of Pennington and Kobe⁵, using the units and symbolism of Herzberg⁶.

$$W_o = W_e - 2W_e X_e$$

$$D_o = 4(Be)^3 / (W_e)^2$$

$$X = W_e X_e / W_e$$

$$B_o = B_e - (1/2)A_e$$

$$s = 2D_o k / (B_o^2 h)$$

$$r = \frac{A_e}{B_e} \left(1 + \frac{A_e}{B_e} \right)$$

$$\frac{F_{rot+to}}{T} = (3/2)R \ln M_w - R \ln \frac{hc B_o}{k} - R \ln \sigma - 7.28295$$

$$\frac{H_{rot+to}}{T} = (7/2)R$$

Vibration contribution

$$U_o = \frac{hc W_o}{kT}$$

$$\frac{F_v}{T} = -R \ln \left(1 - e^{-U_o} \right)$$

$$\frac{H_v}{T} = \frac{RU_o}{e^{U_o} - 1}$$

Electronic contribution

$$U_i = \frac{hc T_i}{kT}$$

$$Q_e = g_o + \sum_i g_i e^{-U_i}$$

$$\frac{F_e}{T} = R \ln Q_e$$

$$\frac{H_e}{T} = \frac{R}{Q_e} \left(\sum_i g_i U_i e^{-U_i} \right)$$

Pennington and Kobe corrections

$$\phi_1 = \frac{1}{e^{U_0} - 1}$$

$$\phi_2 = \frac{U_0 e^{U_0}}{(e^{U_0} - 1)^2}$$

$$\phi_4 = \frac{2U_0}{(e^{U_0} - 1)^2}$$

$$\phi_5 = \frac{(2U_0 (2U_0 e^{U_0} - e^{U_0} + 1))}{(e^{U_0} - 1)^3}$$

$$\frac{F_c}{T} = R(sT + r\phi_1 + \chi\phi_4)$$

$$\frac{H_c}{T} = R(sT + r\phi_2 + \chi\phi_5)$$

$$\frac{F^0 - H^0}{T} = -(7/2)R \ln T - \frac{F_c}{T} - \frac{F_{rotto}}{T} - \frac{F_e}{T} - \frac{F_v}{T}$$

$$H^0 - H^0 = H_v + H_{rotto} + H_c + H_e$$

POLYATOMIC GAS

The harmonic-oscillator rigid rotator approximation is used to compute the thermodynamic functions⁷.

Vibration contribution

$$U_i = \frac{h\nu_i}{kT}$$
$$\frac{F_v}{T} = R \left[\sum_i d_i \ln(1 - e^{-U_i}) \right]$$
$$H_v = RT \sum_i \frac{d_i U_i e^{-U_i}}{1 - e^{-U_i}}$$

Translation contribution

$$\frac{F_t}{T} = - (5/2)R \ln T - (3/2)R \ln M_w - R \ln \left[\left(\frac{2\pi}{N} \right)^{(3/2)} \frac{k^{(5/2)}}{h^3} \right] + R \ln P$$
$$H_t = (5/2)RT$$

Rotation contribution

Non-Linear

$$\frac{F_r}{T} = - (3/2)R \ln T - \frac{R}{2} \ln (I_A I_B I_C) + R \ln \sigma - \ln \left[\pi \left(\frac{k}{hc} \right)^3 + 3 \right] + (3/2)R$$
$$H_r = (3/2)RT$$

Linear

$$\frac{F_r}{T} = - R \ln T - R \ln \frac{k}{hc} - R \ln I_A + R \ln \sigma$$
$$H_r = RT$$

$$\frac{F^{\circ} - H^{\circ}}{T} = \frac{F_r}{T} + \frac{F_v}{T} + \frac{F_t}{T}$$

$$H^{\circ} - H^{\circ}_0 = H_r + H_v + H_t$$

MOMENT OF INERTIA

The moments of inertia are calculated by the method of J. O. Hirschfelder⁸.

The moments of inertia are the eigenvalues of the symmetric matrix:

$$\begin{pmatrix} A & -D & -E \\ -D & B & -F \\ -E & -F & C \end{pmatrix}$$

where

$$Mw = \sum_i m_i$$

$$A = \sum_i m_i (y_i^2 + z_i^2) - \frac{1}{Mw} \left(\sum_i m_i y_i \right)^2 - \frac{1}{Mw} \left(\sum_i m_i z_i \right)^2$$

$$B = \sum_i m_i (x_i^2 + z_i^2) - \frac{1}{Mw} \left(\sum_i m_i x_i \right)^2 - \frac{1}{Mw} \left(\sum_i m_i z_i \right)^2$$

$$C = \sum_i m_i (x_i^2 + y_i^2) - \frac{1}{Mw} \left(\sum_i m_i x_i \right)^2 - \frac{1}{Mw} \left(\sum_i m_i y_i \right)^2$$

$$D = \sum_i m_i x_i y_i - \frac{1}{Mw} \left(\sum_i m_i x_i \right) \left(\sum_i m_i y_i \right)$$

$$E = \sum_i m_i x_i z_i - \frac{1}{Mw} \left(\sum_i m_i x_i \right) \left(\sum_i m_i z_i \right)$$

$$F = \sum_i m_i y_i z_i - \frac{1}{Mw} \left(\sum_i m_i y_i \right) \left(\sum_i m_i z_i \right)$$

The moments of inertia are then multiplied by 1.66035×10^{-1} to get the proper mass units for use in the polyatomic thermodynamic function code.

ONE DEBYE THETA SOLID

The formulas for the Debye approximation are given by Menzel⁹ and Trasov¹⁰. The Debye integral is done numerically using Simpson's Rule and 1000 intervals.

$$x = \frac{\theta}{T}$$

$$D(x) = \frac{M}{x^M} \int_0^x \frac{x^M dx}{e^x - 1}$$

$$\frac{F^0 - H_0^0}{T} = SR[M \ln(1 - e^{-x}) + (2-M)D(x)]$$

$$H^0 - H_0^0 = 3SRD(x)$$

$$C_v = 3SR \left[(M+1)D(x) - \frac{Mx}{e^x - 1} \right]$$

TWO DEBYE THETA SOLID

The theory of the calculation is described by Krumhansl and Brooks¹¹.

$M = 2$, 2 dimensional

$$x_t = \frac{\theta}{T} t$$

$$x_l = \frac{\theta}{T} l$$

$$D(x) = \frac{M}{x^M} \int_0^x \frac{x^M dx}{e^x - 1}$$

$$\frac{F^0 - H_0^0}{T} = SR \left[\frac{1}{2} \left((1-M)D(x_t) - M \ln(1 - e^{-x_t}) \right) + (1-M)D(x_l) - M \ln(1 - e^{-x_l}) \right]$$

$$H^0 - H_0^0 = 2SRT \left(\frac{1}{2} D(x_t) + D(x_l) \right)$$

$$C_v = 2SR \left[\frac{1}{2} \left((M+1)D(x_t) - \frac{Mx_t}{e^{x_t} - 1} \right) + (M+1)D(x_l) - \frac{Mx_l}{e^{x_l} - 1} \right]$$

GENERAL

In all cases the entropy is calculated from the equation.

$$S^{\circ} = \frac{H^{\circ} - H_{\circ}^{\circ}}{T} - \frac{F^{\circ} - H_{\circ}^{\circ}}{T} .$$

The integration constant is calculated from the fit on S° as follows:

$$IC = H^{\circ} - H_{\circ}^{\circ} - \int T \frac{\partial S}{\partial T} dT$$

S° is fit to $S^{\circ} = A + BT + CT^2 + DT^3 + ET^5$, then

$$IC = H^{\circ} - H_{\circ}^{\circ} - \left[\frac{BT^2}{2} + \frac{2CT^3}{3} + \frac{3}{4} DT^4 + \frac{4}{5} ET^5 \right]$$

NOMENCLATURE

Mw	Molecular weight in grams/mole
T	Temperature in °K
σ	Symmetry number
h	Plank's constant (6.62377×10^{-27} erg sec)
c	Speed of light (2.997902×10^{10} cm/sec)
k	Boltzmann's constant (1.380257×10^{-16} erg/deg)
R	Gas constant (1.98719 cal/deg mole)
T_i	Term value of i^{th} electronic state (1/cm)
g_i	Statistical weight of i^{th} electronic state
We	Vibrational frequency (1/cm)
WeXe	Anharmonic coefficient (1/cm)
Be	Rotational coefficient (1/cm)
Ae	Rotational-Vibrational coefficient (1/cm)
ν_i	Fundamental frequency (1/cm)
d_i	Degeneracy of fundamental frequency
I_A, I_B, I_C	Moments of Inertia ($\text{gm-cm}^2 \times 10^{39}$)
m_i	Atomic weight of i^{th} atom (amu)
x_i, y_i, z_i	Cartesian coordinates of i^{th} atom (Å)
N	Avogadro's number [6.0238×10^{23} (gm-mole) $^{-1}$]
P	One atmosphere of pressure
M	Dimension (1, 2, or 3)
S	Number of atoms per cell
θ	Debye temperature (°K)
θ_t	Debye temperature transverse (°K)
θ_l	Debye temperature longitudinal (°K)

$\frac{F^{\circ} - H^{\circ}}{T}$ Free energy function (cal/mole/°K)

$H^{\circ} - H^{\circ}_0$ Enthalpy (cal/mole)

S° Entropy (cal/mole/°K)

C_v Heat Capacity (cal/mole/°K)

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