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A VIRIAL EQUATION OF STATE OPTION
FOR THE TIGER COMPUTER PROGRAM

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Aivars K.R. Celmins

October 1984

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20 ABSTRACT (Continue on reverse side if necessary and identify by block number) REF This report describes a truncated virial equation of state option for the TIGER computer program which computes thermodynamic properties of systems of gases, liquids and solids. The second virial coefficients of the added equation is based on Lennard-Jones (6-12) intermolecular potential, whereas the third virial coefficient is derived from a simplified rigid sphere approximation. This report provides an outline of the derivation of the pertinent formulas and a listing of the added subroutines. The listing (Continued on reverse side)		

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20. ABSTRACT (Continued)

contains numerous comments that may be useful for a preparation of other gaseous state equations for the TIGER program.

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TABLE OF CONTENTS

	<u>Page</u>
1. INTRODUCTION.....	5
2. PRINCIPAL RESULTS.....	5
3. USER'S GUIDE FOR THE SUBROUTINE LJ612.....	8
4. EXAMPLE OF A COMPUTATION.....	10
5. DERIVATION OF PRINCIPAL FORMULAS.....	10
6. COMPUTATION OF SECOND VIRIAL COEFFICIENTS.....	14
7. COMPUTATION OF THIRD VIRIAL COEFFICIENTS.....	17
8. SUMMARY AND CONCLUSION	18
ACKNOWLEDGEMENT.....	19
REFERENCES.....	20
APPENDIX A. Listing of the Subroutine LJ612.....	21
APPENDIX B. Listing of the Subroutine LJBS.....	35
APPENDIX C. Sample Output.....	41
APPENDIX D. Interpolation Formulas.....	53
DISTRIBUTION LIST.....	59



A1

1. INTRODUCTION

This report describes a supplement to the TIGER computer program.¹ The latter is a program for the calculation of thermodynamic properties of nonideal systems of specified atomic compositions containing gaseous, liquid and solid phases with known equations of state. The TIGER program version that is documented in Ref. 1 has options to use for the gaseous constituents either the ideal equation of state or one of three nonideal equations. The latter three are called BKW (Becker, Kistiakowsky and Wilson), JCZ1 and JCZ2 (Jacobs, Cowperthwaite and Zwisler), respectively, and defined in Ref. 1. The present report describes a modification of the TIGER program which permits one to also use a fifth gaseous state equation, namely, a truncated virial equation in which the second virial coefficient is determined from Lennard-Jones (6-12) potential parameters. The added equation of state subroutine has been given the name LJ612 in order to indicate its relation to the Lennard-Jones potential. The principal features of the added equation of state are described in Section 2, and control cards that activate the routine LJ612 are discussed in Section 3. Section 4 gives a sample calculation. Details of the derivation of the pertinent equations and formulas are given in Sections 5, 6 and 7. These details should be of interest to users of the LJ612 option if the basic equations are modified, for instance, for numerical expediency. In order to facilitate such a modification the subroutines LJ612 and LJBS (an auxiliary routine) are listed in Appendices A and B, respectively, with numerous explanatory comments. These comments make the listing of LJ612 also useful as a guide for the preparation of other nonideal equations of state routines. Section 8 contains a summary and conclusion.

In order to use the subroutine LJ612 in the TIGER program, the subroutine STATEG must be changed as described in Ref. 1, p. III-C-348. That change merely increases by one the number of available gaseous equations of state and includes a call to the added subroutine LJ612 at the proper place. No other changes in the TIGER program are needed.

2. PRINCIPAL RESULTS

The modifications of the TIGER program permit one to use the following type of equation of state for gases:

$$p = \frac{RT}{\tilde{V}} \phi(\tilde{V}, T) \quad (2.1)$$

¹M. Cowperthwaite and W. H. Zwisler, "TIGER Computer Program Documentation," Stanford Research Institute Publication Z106, January 1973.

with

$$\phi(\tilde{V}, T) = 1 + \frac{B(T)}{\tilde{V}} + \frac{C}{\tilde{V}^2} \quad (2.2)$$

In these equations, p (Pa) is the pressure, $R = 8.3143 \text{ J/(K}\cdot\text{mol)}$ is the universal gas constant, T (K) is temperature, $\tilde{V}$ (m^3/mol) is the molar volume, ϕ is the imperfection parameter, B (m^3/mol) is the second virial coefficient, and C (m^6/mol^2) is the third virial coefficient. The formula (2.2) for ϕ is called a truncated virial form because it can be considered as the first three terms of an infinite series expansion with terms of the type $A_K(T)/\tilde{V}^K$. The second virial coefficient $B(T)$ in Eq. (2.2) is computed assuming that the intermolecular forces have the empirical potential function

$$\phi(r) = 4 \epsilon [(\sigma/r)^{12} - (\sigma/r)^6] \quad (2.3)$$

where r (m) is the distance between molecules, and ϵ (J) and σ (m) are parameters characteristic of each gas (Ref. 2, p. 32). The function defined by Eq. (2.3) is called the Lennard-Jones (6-12) potential. σ is that value of r for which $\phi(r) = 0$, and ϵ is the maximum energy of attraction (or depth of the potential well) which occurs at $r = 2^{1/6}\sigma = 1.12\sigma$. Typical values of σ are around $3.5 \cdot 10^{-10}$ m. The parameter ϵ enters the present calculations only in the ratio ϵ/k , where $k = 1.38054 \cdot 10^{-22} \text{ J/K}$ is the Boltzmann constant. Typical values of the ratio ϵ/k are around 300 K.

For a single gas with given σ and ϵ/k the second virial coefficient $B(T)$ is calculated as follows. (Ref. 2, p. 162 ff.). First, one defines a dimensionless reduced temperature T^* by

$$T^* = T k / \epsilon \quad (2.4)$$

and a reduced dimensionless coefficient B^* by

$$B^* = B / b_0(\sigma) \quad (2.5)$$

where

²J.O. Hirschfelder, C.F. Curtiss and R.B. Bird, "Molecular Theory of Gases and Liquids," John Wiley and Sons, New York, 1954.

$$b_0(\sigma) = \frac{2}{3} \pi \tilde{N} \sigma^3, \quad (2.6)$$

and $\tilde{N} = 6.02252 \cdot 10^{23} \text{ mol}^{-1}$ is the Avogadro number. $\tilde{B}$ is for a given intermolecular potential function of Lennard-Jones type a unique function of T . It can be calculated by a series expansion and it is tabulated for the Lennard-Jones (6-12) potential in Ref. 2, p. 1114 ff. The relation between B , T , σ and ϵ is in terms of the function $\tilde{B}$ as follows

$$B(T) = b_0(\sigma) \cdot \tilde{B}(T k/\epsilon) \quad (2.7)$$

For gas mixtures the computation of $B(T)$ is modified such that in Eq. (2.7) one uses for σ and ϵ averages of the parameters of pairs of individual constituents, and computes the final $B(T)$ by averaging over all pairs. Details of the calculation of $B(T)$ are given in Sections 5 and 6.

A corresponding computation of the third virial coefficient C for gases with Lennard-Jones potential is described on Ref. 2, pp. 150 ff., 170 ff., 228 ff. and 1119. The algorithm is complicated and the resulting C is not accurate. Therefore, instead of using the Lennard-Jones potential, the third virial coefficient computation for a single gas is for the present task based on a rigid sphere approximation from Ref. 2, p. 157:

$$C(\sigma) = \frac{5}{8} b_0^2(\sigma) \cdot 0.81^6, \quad (2.8)$$

where $b_0(\sigma)$ is given by Eq. (2.6). To simplify further, the third virial coefficient for mixtures of gases is computed by a simple averaging of the individual values of C , described in Section 5. Hirschfelder et al.² p. 153, derive a more complicated formula but considering the large uncertainties of the result, the simpler averaging was deemed to be adequate. This computation of the third virial coefficient was suggested by E. Freedman and it is implemented in the BLAKE computer program.³ The factor 0.81^6 is empirical and suggested in Ref. 2, p. 157. It may be replaced by a different factor, as described in Section 3.

³F. Freedman "BLAKE - a Thermodynamics Code Based on TIGER: User's Guide and Manual," ARBRL-TR-02411, July 1982. AD# A121259.

In summary, the supplemented TIGER program can be used with the equation of state (2.1) and (2.2) for gases. The user should supply for each gaseous constituent of the system the proper values of σ and ϵ of the Lennard-Jones (6-12) potential parameters. If such are not supplied and also not already stored in the TIGER file of material constants, then the LJ612 routine uses the following default values:

$$\sigma = 3.5 \cdot 10^{-10} \text{ m ,}$$

(2.9)

$$\epsilon/k = 300 \text{ K .}$$

3. USER'S GUIDE FOR THE SUBROUTINE LJ612

The virial equation of state supplement LJ612 of the TIGER program can be activated by the same type of control cards as the other four equations of state. Particulars of input data and order are provided in Ref. 1. This section supplements that reference, particularly its Volume IV, "User's Guide of the TIGER Computer Program."

The instruction to use the LJ612 equation of state is given by a GEOS-card which has the format

GEOS,LJ612

(see Ref. 1, IV-C-10-11). The card instructs the TIGER program to use the LJ612 equation of state for all computations until another GEOS card is encountered in the input. Therefore, it should be placed in the input deck before any of the instruction cards that initiate a computation, that is, before POINT, ISOLINE, GRID, EXPLOSION, C-J CONDITION or HUGONIOT cards.

The empirical factor 0.81 that enters Eq. (2.8) for the third virial coefficient can be changed by a SET-card. (See Ref. 1, IV-C-18). The card has the format

SET,LJ612,SFACT,a

where "a" is the number that replaces the value 0.81 in Eq. (2.8). For instance, if $a = 0$, then $C = 0$ and the virial Eq. (2.2) is truncated to two terms. The SET-card should of course precede all the calculation instruction cards listed above. Once the factor has been set then it remains in effect for the particular TIGER run until changed by another SET-

card.

The Lennard-Jones (6-12) potential parameters σ and ϵ/k are provided by a STG-card for each gaseous constituent. These cards are used in a TIGER run that updates (replaces) the TIGER file containing material constants. The input and instruction cards for such a run are described in Ref. 1, IV-C-24 ff. For a gaseous constituent with the designation "name" the input consists of the following sequence (see Ref. 1, IV-C-25):

```
CONSTITUENT,name,GAS
STR,name,GAS,1, . . .
STR,name,GAS,2, . . .
STR,name,GAS,3, . . .
STG,LJ612,name, $\sigma$ ,  $\epsilon/k$ 
```

Other STG-cards specifying constants for the BKW, JC22 or JC23 equations of state may follow or precede the STG,LJ612-card. The next card after the STG-cards is another CONSTITUENT-card. The value of σ must be entered in 10^{-10} m (in ångströms) and the value of ϵ/k should be expressed in kelvins. An example of a STG-card is

```
STG,LJ612,H2O,2.79,542.5
```

indicating that for the constituent called H2O the Lennard-Jones potential parameters are $\sigma = 2.79 \cdot 10^{-10}$ m and $\epsilon/k = 542.5$ K. If either σ or ϵ/k is negative or zero in the STG-card, then the corresponding default value ($\sigma = 3.5 \cdot 10^{-10}$ m, $\epsilon/k = 300$ K) is stored in the library file instead of the negative or zero value from the card. If the library file does not contain values of the Lennard-Jones potential parameters for a constituent, then default values are generated as needed by the subroutine LJ612 at run time. (That is, if the LJ612 is activated by a GEOS,LJ612-card and the constituent is part of the system that is evaluated.) The contents of the library file are not affected by such computations.

More details of the structure and operation of the subroutine LJ612 and the auxiliary routine LJBS are provided by comments in the listings of the routines in Appendices A and B, respectively.

4. EXAMPLE OF A COMPUTATION

We chose as an example for the operation of the LJ612 equation of state routine the same problem as in Ref. 1, p. IV-E-17 ff. The present input differs from that in Ref. 1 only by the GEOS-card. The output is given in Appendix C. Comparison of the output with that of Ref. 1 shows two types of differences. First, one observes the expected difference in values for temperature, pressure and other thermodynamic variables, because a different equation of state was used. However, in addition to these changes, and, possibly masking the effect of the equation of state, there is also a change of the composition of the gas. This change is not a consequence of the new equation of state but rather of the evolution of the TIGER library data between the publication of Ref. 1 and its present version.

5. DERIVATION OF PRINCIPAL FORMULAS

We consider an equation of state of the form

$$p = \frac{RT}{\tilde{V}} \phi(\tilde{V}, T) \quad (5.1)$$

where

$$\phi(\tilde{V}, T) = 1 + \frac{B(T)}{\tilde{V}} + \frac{C}{\tilde{V}^2} \quad (5.2)$$

In the TIGER program, the molar volume $\tilde{V}$ is not directly used as a variable. Instead, it may be calculated from the following relations (Ref. 1, p. I-B-16):

$$\tilde{V} = \frac{1}{n} V = \frac{1}{n} \frac{M_g}{\rho} = \frac{1}{n} \frac{M_o}{\hat{\rho}} \quad (5.3)$$

where n is the number of moles, V is the gas volume, M_g is the mass of the gas, ρ is its density and M_o is the mass of the mixture. The density $\hat{\rho}$ is defined as the mass of the mixture divided by the volume of the gas. The quantities n , M_o and $\hat{\rho}$ are TIGER variables from which $\tilde{V}$ may be computed. Let the system have s gaseous constituents with mole numbers n_i , $i=1, \dots, s$. Then

$$n = \sum_{i=1}^s n_i \quad (5.4)$$

The n_i are also TIGER variables. The equation of state is in terms of these variables.

$$p = R T n \frac{\hat{\phi}}{M_0} \quad (5.5)$$

with

$$\begin{aligned} \hat{\phi} &= \hat{\phi}(p, T, M_0, n_1, n_2, \dots, n_s) \\ &= 1 + \frac{\hat{p}}{M_0} n B(T, n_1, \dots, n_s) + \left(\frac{\hat{p}}{M_0}\right)^2 n^2 C(n_1, \dots, n_s) \end{aligned} \quad (5.6)$$

The virial coefficients B and C depend on the mole numbers n_i of the individual constituents because they represent the non-ideal effect of all s constituents and the n_i specify the quality of the mixture. Both coefficients also depend on the individual Lennard-Jones potential parameters σ_i and ϵ_i , in a form that will be shown shortly.

The second virial coefficient B is calculated for a system of gases by the formula (Ref. 2, p. 153)

$$B = \frac{1}{n^2} \sum_{i=1}^s \sum_{j=1}^s n_i n_j B_{ij} \quad (5.7)$$

In this formula the B_{ij} are the second virial coefficients of a potential function which describes the interaction between molecules of constituent i and constituent j . They are functions of the form

$$B_{ij} = B_{ij}(T, \sigma_i, \sigma_j, \epsilon_i/k, \epsilon_j/k) \quad (5.8)$$

that is, they depend on the gas temperature T and on the Lennard-Jones potential parameters of both constituents. The calculation of the B_{ij} will be described in Section 6.

The third virial coefficient C in Eq. (5.6) is computed as the average

$$C = \frac{1}{n} \sum_{i=1}^s n_i C_i \quad (5.9)$$

of the third virial coefficients C_i of the individual constituents. The latter are assumed to be independent of temperature and ϵ_i , that is,

$$C_1 = C_1(\sigma_1) \quad (5.10)$$

The calculation of the C_1 is based on a rigid sphere approximation. (See Section 7).

In order to simplify the following formulas, we define

$$\sum_B = \sum_{i=1}^S \sum_{j=1}^S n_i n_j B_{ij} \quad (5.11)$$

$$\sum_B' = \sum_{i=1}^S \sum_{j=1}^S n_i n_j \frac{dB_{ij}}{dT} \quad (5.12)$$

$$\sum_B'' = \sum_{i=1}^S \sum_{j=1}^S n_i n_j \frac{d^2 B_{ij}}{dT^2} \quad (5.13)$$

and

$$\sum_C = \sum_{i=1}^S n_i C_i \quad (5.14)$$

The imperfection parameter ϕ is given in terms of these quantities by

$$\phi = 1 + \frac{\hat{p}}{M_0} \frac{1}{n} \sum_B + \left(\frac{\hat{p}}{M_0}\right)^2 n \sum_C \quad (5.15)$$

The TIGER program carries out a number of different computations for which it needs in addition to the value of the imperfection parameter ϕ also the values of certain expressions involving ϕ . These expressions are calculated in the equation of state subroutines. Next, we shall derive formulas for these quantities. (See Ref. 1, p. II-C-11).

First, there are three derivatives of ϕ :

$$\frac{\partial \ln \phi}{\partial \ln \hat{p}} = \frac{\hat{p}}{\phi} \frac{\partial \phi}{\partial \hat{p}} = \frac{1}{\phi} \left(\frac{\hat{p}}{M_0} \frac{1}{n} \sum_B + 2 \left(\frac{\hat{p}}{M_0} \right)^2 n \sum_C \right) \quad (5.16)$$

$$\frac{\partial \ln \phi}{\partial \ln T} = \frac{T}{\phi} \frac{\partial \phi}{\partial T} = \frac{1}{\phi} \frac{\hat{p}}{M_0} \frac{1}{n} T \sum_B' \quad (5.17)$$

and

$$\frac{\partial \ln \phi}{\partial n_i} = \frac{1}{\phi} \frac{\partial \phi}{\partial n_i} = \frac{1}{\phi} \left\{ \frac{1}{n} \left[-\frac{\hat{p}}{M_o} \frac{1}{n} \right]_B + \left(\frac{\hat{p}}{M_o} \right)^2 n \left[C \right] + \right. \\ \left. + \frac{\hat{p}}{M_o} \frac{2}{n} \sum_{j=1}^S n_j B_{ij} + \left(\frac{\hat{p}}{M_o} \right)^2 n C_i \right\} \quad (5.18)$$

Notice that the first two expressions, Eqs. (5.16) and (5.17), are dimensionless; whereas, the expression (5.18) has the dimension 1/mol. Another dimensionless quantity is

$$\Gamma_i = \int_0^{\hat{p}} \left[\frac{M_o}{R T \hat{p}} \frac{\partial p}{\partial n_i} - 1 \right] \frac{d\hat{p}}{\hat{p}} = \int_0^{\hat{p}} \left[\frac{\partial (n\phi)}{\partial n_i} - 1 \right] \frac{d\hat{p}}{\hat{p}} - \\ = \int_0^{\hat{p}} \left[\phi - 1 + n \frac{\partial \phi}{\partial n_i} \right] \frac{d\hat{p}}{\hat{p}} \quad (5.19)$$

An evaluation of the integral (5.19) yields for Γ_i the formula

$$\Gamma_i = 2 \frac{\hat{p}}{M_o} \sum_{j=1}^S n_j B_{ij} + \frac{1}{2} \left(\frac{\hat{p}}{M_o} \right)^2 n^2 C_i + \left(\frac{\hat{p}}{M_o} \right)^2 n \left[C \right] \quad (5.20)$$

Other expressions needed by the TIGER program are the following two dimensionless derivatives of Γ_i :

$$\frac{\partial \Gamma_i}{\partial \ln \hat{p}} = \hat{p} \frac{\partial \Gamma_i}{\partial \hat{p}} = 2 \frac{\hat{p}}{M_o} \sum_{j=1}^S n_j B_{ij} + \left(\frac{\hat{p}}{M_o} \right)^2 n^2 C_i + 2 \left(\frac{\hat{p}}{M_o} \right)^2 n \left[C \right] \quad (5.21)$$

and

$$\frac{\partial \Gamma_i}{\partial \ln T} = T \frac{\partial \Gamma_i}{\partial T} = 2 \frac{\hat{p}}{M_o} \sum_{j=1}^S n_j T \frac{dB_{ij}}{dT} \quad (5.22)$$

and the following derivative with the dimension 1/mol

$$\frac{\partial \Gamma_i}{\partial n_j} = 2 \frac{\hat{p}}{M_o} B_{ij} + \left(\frac{\hat{p}}{M_o} \right)^2 \left[\left[C \right] + n (C_i + C_j) \right] \quad (5.23)$$

The next two quantities have the dimension of moles and are defined by

$$\epsilon = \int_0^{\hat{p}} \frac{M_0}{R T \hat{p}} \left(p - T \frac{\partial p}{\partial T} \right) \frac{d\hat{p}}{\hat{p}} = - \int_0^{\hat{p}} T \frac{\partial(n\phi)}{\partial T} \frac{d\hat{p}}{\hat{p}} \quad (5.24)$$

and

$$\epsilon_T = - \int_0^{\hat{p}} \frac{M_0 T}{R \hat{p}} \frac{\partial^2 p}{\partial T^2} \frac{d\hat{p}}{\hat{p}} = \frac{\partial(\epsilon T)}{\partial T} \quad (5.25)$$

An evaluation of these expressions yields

$$\epsilon = \frac{\hat{p}}{M_0} T \tau_B' \quad (5.26)$$

and

$$\epsilon_T' = - \frac{\hat{p}}{M_0} \left(2 T \tau_B' + T^2 \tau_B'' \right) \quad (5.27)$$

We notice that the quantity ϵ that is defined by Eq. (5.24) or (5.26) is an auxiliary variable for the TIGER program and not the Lennard-Jones potential parameter ϵ .

In order to evaluate the expressions (5.15) through (5.18), (5.20) through (5.23), (5.26) and (5.27), one needs values for the virial coefficients B_{ij} and its temperature derivatives which enter the formulas in the combinations $T \cdot dB_{ij}/dT$ and $T^2 \cdot d^2 B_{ij}/dT^2$, and the virial coefficients C_i . The computation of the former three is treated in the next section. The computation of the C_i is described in Section 7.

6. COMPUTATION OF SECOND VIRIAL COEFFICIENTS

The second virial coefficient B_{ij} in Eq. (5.7) represents the interaction between molecules of constituent i and constituent j . It may be computed as the virial coefficient of a pure substance with an intermolecular potential that is an empirical combination of the potential functions of both constituents. In this report, we use the following empirical combining rules to specify the constants σ_{ij} and ϵ_{ij} of the mixture potential (Ref. 2, p. 168, Ref. 3, p. 11):

$$\sigma_{ij} = \frac{1}{2} (\sigma_i + \sigma_j) \quad (6.1)$$

and

$$\frac{\epsilon_{ij}}{k} = \left(\frac{\sigma_i}{\sigma_{ij}} \cdot \frac{\sigma_j}{\sigma_{ij}} \right)^{3/2} \left(\frac{\epsilon_i}{k} \cdot \frac{\epsilon_j}{k} \right)^{1/2} \quad (6.2)$$

We notice that for $i=j$ these formulas produce $\sigma_{ii} = \sigma_i$, $\epsilon_{ii} = \epsilon_i$ and, consequently, $B_{ii} = B_i$. The σ_{ij} and ϵ_{ij} are treated as the Lennard-Jones (6-12) potential parameters of a pure substance and B_{ij} is computed as the second virial coefficient of that substance. This is done by defining a dimensionless reduced temperature T^* and computing a corresponding dimensionless virial coefficient $B(T^*)$ from which B_{ij} then can be retrieved. The function $B(T)$ is uniquely determined by the constants of the Lennard-Jones potential. The following formulas are used to carry out this calculation:

$$T^* = T k / \epsilon_{ij} \quad , \quad (6.3)$$

$$b_{oij} = \frac{2}{3} \pi \tilde{N} \sigma_{ij}^3 \quad , \quad (6.4)$$

$$B_{ij} = b_{oij} B(T^*) \quad , \quad (6.5)$$

where $\tilde{N} = 6.02252 \cdot 10^{23} \text{ mol}^{-1}$ is the Avogadro constant.

The function $B(T)$ is defined by the following infinite series (Ref. 2, p. 163):

$$B(T) = \sum_{m=0}^{\infty} b_m T^m (-1/4 - m/2) \quad (6.6)$$

with

$$b_m = - \frac{2^m \sqrt{\pi}}{4 \cdot m!} \Gamma(-\frac{1}{4} + \frac{1}{2} m) \quad (6.7)$$

The first two coefficients in the series (6.6) are⁴

⁴P. Jahnke and E. Emde, "Tables of Higher Functions," B.G. Teubner, Leipzig 1948.

$$b_0 = -\frac{\sqrt{2}}{4} \Gamma(-\frac{1}{4}) = \sqrt{2} \cdot 1.225\ 416\ 702\ 7 \quad (6.8)$$

and

$$b_1 = -\frac{\sqrt{2}}{2} \Gamma(\frac{1}{4}) = -\frac{\sqrt{2}}{2} \cdot 3.625\ 609\ 908 \quad (6.9)$$

All other coefficients can be calculated from b_0 and b_1 by the recurrence formula

$$b_{m+2} = b_m \frac{2m-1}{(m+1)(m+2)}, \quad m = 0, 1, 2, \dots \quad (6.10)$$

We rearrange the series (6.6) as follows for arithmetical expediency

$$\begin{aligned} {}^*B(T) &= \sum_{m=0}^{\infty} [b_{2m} \frac{1}{T} (-1/4 - m) + b_{2m+1} \frac{1}{T} (-3/4 - m)] \\ &= \sum_{m=0}^{\infty} (A_{0,m} + A_{1,m}) \end{aligned} \quad (6.11)$$

The $A_{0,m}$ and $A_{1,m}$ are defined by

$$A_{0,0} = b_0 \frac{1}{T} (-1/4) \quad (6.12)$$

$$A_{1,0} = b_1 \frac{1}{T} (-3/4) \quad (6.13)$$

and by the recurrence formulas for $m = 0, 1, 2, \dots$

$$A_{0,m+1} = A_{0,m} \frac{4m-1}{(2m+1)(2m+2)} \cdot \frac{1}{\frac{1}{T}} \quad (6.14)$$

$$A_{1,m+1} = A_{1,m} \frac{4m+1}{(2m+2)(2m+3)} \cdot \frac{1}{\frac{1}{T}} \quad (6.15)$$

The series for ${}^*B(T)$ converges absolutely for all $|T| > 0$. Therefore, one can compute the derivatives of ${}^*B(T)$ by termwise differentiation which produces the following formulas

$$\frac{d^2 B}{dT^2} = \sum_{m=0}^{\infty} \left(-\frac{4m+1}{4} A_{0,m} - \frac{4m+3}{4} A_{1,m} \right) \quad (6.16)$$

and

$$\frac{d^2 B}{dT^2} = \sum_{m=0}^{\infty} \left[\frac{(4m+1)(4m+5)}{16} A_{0,m} + \frac{(4m+3)(4m+7)}{16} A_{1,m} \right] \quad (6.17)$$

The evaluation of the series (6.11), (6.16) and (6.17) is done in the subroutine LJBS which computes for given T the corresponding values of B , $T B'$ and $T^2 B''$. The series converge very fast if T is large, but require the computation of a large number of terms if T is small. Typical TIGER computations are done with values of T between one and two. In that range some computation time can be saved by interpolating $B(T)$ and its derivatives in tables instead of evaluating the series. Such tables are published in Ref. 2, p. 1144 ff., Tables I-B. The subroutine LJBS uses these tables for the computation of B and its derivatives by interpolation if T is within the range (0.75, 5.0). If $T = 5.0$, then only six to seven terms of the series have to be calculated, and the number of terms decreases as T increases. (The end criterion for the series calculation in LJBS is that the absolute value of the last term is less than 10^{-12} .) On the other hand, if $T < 0.75$ then the table interpolation is not very accurate due to rapid changes of the functions. Therefore, within the range (0.01, 0.75) again the series formulas are used. The number of terms that have to be evaluated is 350 at $T = 0.01$. However, one would not expect typical TIGER calculations to be done for $T < 0.75$. For $T < 0.01$ an error stop with a corresponding printed message is programmed into LJ612.

The interpolation in the tables is done by Hermite interpolation formulas which make use of the availability of the derivatives of the interpolated functions. Particulars about the interpolation formulas are given in Appendix D.

In a limited number of test runs the computing time that was saved by interpolation was found to be of the order of two percent.

7. COMPUTATION OF THIRD VIRIAL COEFFICIENTS

The third virial coefficient C is computed by Eq. (5.9) as an average of the third virial coefficients C_i of the individual constituents. The latter coefficients we compute from a rigid sphere approximation. According to Ref. 2, p. 157, a reasonable value for C_i in case of high temperature powder gases is

$$C_1 = \frac{5}{8} \left(\frac{2}{3} \pi \tilde{N} \right)^2 (0.81 \cdot \sigma_1)^6 \quad (7.1)$$

where $\tilde{N} = 6.02252 \cdot 10^{23} \text{ mol}^{-1}$ is the Avogadro constant and σ_1 is the Lennard-Jones (6-12) potential parameter. The factor 0.81 in Eq. (7.1) is an approximation to the theoretical value for the Lennard-Jones potential at $T^* \approx 60$. (See Eqs. (2.4) and (6.3) for the definition of the reduced temperature T^* .) Theoretically the factor may be increased to about 0.99 for $T^* = 1.25$ (as can be seen from Ref. 2, pp. 171 and 1116 - 1117). However, experimental measurements deviate considerably from the theoretical value and, therefore, the constant 0.81 likely suffices to establish a correct order of magnitude effect of the third virial coefficients on TIGER calculations. If necessary, the factor can be changed for any particular calculations by using the SET-card. (See Section 3). Particularly, by setting the factor equal to zero and repeating the calculation one can obtain the total effect of the third virial coefficients on the calculated results.

8. SUMMARY AND CONCLUSION

This report describes two new subroutines that can be included in the TIGER computer program and enables the latter to do computations using a truncated virial equation of state for the gaseous constituents. The second virial coefficient in the equation is based on Lennard-Jones (6-12) intermolecular potential, and the third virial coefficient is based on a simplified rigid sphere assumption. The new equation of state subroutine is called LJ612. It uses an auxiliary subroutine LJBS which computes a function B and its derivatives for given T . The latter is a reduced dimensionless temperature and B is a dimensionless second virial coefficient for Lennard-Jones (5-12) potential and pure substances. The LJ612 subroutine has an option (SET-card) to multiply the third virial coefficient by an arbitrary constant. By setting the constant equal to zero one can obtain an estimate of the significance of the third virial coefficient for any particular computation.

The TIGER program was carefully studied during the programming of the additional routines. It was found that the description of the program in Ref. 1 is not up to date and, particularly, that the comments in the BKW equation of state routine are not complete and sufficient for an easy addition of new equations of state. Therefore, the new subroutine LJ612 was provided with numerous comments which may be helpful for adding another equation of state to the TIGER program. We also notice that although the TIGER program guide claims that input and output data can be easily changed to arbitrary units (Ref. 1, IV-C-4), instructions are not provided how to implement such changes, nor do such changes, if implemented, affect the input information for the equations of state. The internal calculations are

done in prescribed units which were also adopted for the LJ612 subroutine and documented in the comments to LJ612. The information about the units of all quantities is important because some of them ($\partial(\ln \phi)/\partial n_i$, $\partial \Gamma_i/\partial n_i$, ϵ , ϵ_T) are not dimensionless, contrary to statements in the TIGER documentation. Input units for the Lennard-Jones (6-12) potential parameters were chosen to be 10^{-10} m (Ångströms) for σ and kelvins for ϵ/k . A change of these units would require minor changes in the LJ612 subroutine and would not affect the rest of the TIGER program.

In conclusion, the addition of the two subroutines LJ612 and LJBS permits one to use a truncated virial equation of state and, because the routines are carefully commented, facilitates the addition of further gaseous state equations.

ACKNOWLEDGEMENT

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APPENDIX A
LISTING OF THE SUBROUTINE LJ612

APPENDIX A LISTING OF THE SUBROUTINE LJ612

CCCCCCCCCCCCCCCC	SUBROUTINE LJ612(LANE)	LJ612	2
CCCCCCCCCCCCCCCC	PURPOSE	LJ612	3
CCCCCCCCCCCCCCCC	TO COMPUTE THE OUTPUT FOR STATE USING A TRUNCATED	LJ612	4
CCCCCCCCCCCCCCCC	VIRIAL EQUATION OF STATE IN WHICH THE SECOND COEFFICIENT	LJ612	5
CCCCCCCCCCCCCCCC	IS BASED ON LENNARD-JONES 6-12 POTENTIAL AND	LJ612	6
CCCCCCCCCCCCCCCC	THE THIRD COEFFICIENT IS COMPUTED USING A	LJ612	7
CCCCCCCCCCCCCCCC	SIMPLIFIED RIGID SPHERE FORMULA	LJ612	8
CCCCCCCCCCCCCCCC	INPUT AND OUTPUT DEPEND ON THE VALUE OF LANE	LJ612	9
CCCCCCCCCCCCCCCC	INPUT VARIABLES	LJ612	10
CCCCCCCCCCCCCCCC	INPUT FOR LANES 1 THROUGH 4	LJ612	11
CCCCCCCCCCCCCCCC	LO = NUMBER OF OUTPUT UNIT (PRINTER)	LJ612	12
CCCCCCCCCCCCCCCC	NSG = NUMBER OF GASEOUS CONSTITUENTS	LJ612	13
CCCCCCCCCCCCCCCC	RHO = MASS OF MIXTURE PER VOLUME OF GAS IN G/CM**3	LJ612	14
CCCCCCCCCCCCCCCC	THIS IS CALLED RHO-HAT IN TEXT, SEE I-8-16.	LJ612	15
CCCCCCCCCCCCCCCC	SX = SUM OF GASEOUS MOLE NUMBERS X(I), IN MOLES.	LJ612	16
CCCCCCCCCCCCCCCC	T = GAS TEMPERATURE IN KELVINS	LJ612	17
CCCCCCCCCCCCCCCC	#M = REFERENCE MASS IN GRAMS (M=ZERO IN I-8-16)	LJ612	18
CCCCCCCCCCCCCCCC	X(I) = MOLE NUMBER OF THE I-TH GASEOUS CONSTITUENT	LJ612	19
CCCCCCCCCCCCCCCC	WITH I=1,...., NSG, IN MOLES	LJ612	20
CCCCCCCCCCCCCCCC	INPUT FOR LANES 5 AND 6	LJ612	21
CCCCCCCCCCCCCCCC	NONE	LJ612	22
CCCCCCCCCCCCCCCC	INPUT FOR LANE 7	LJ612	23
CCCCCCCCCCCCCCCC	IDEAL = NUMBER OF THIS EQUATION OF STATE	LJ612	24
CCCCCCCCCCCCCCCC	VAL(1) = VALUE OF THE SECOND FIELD OF THE "GEOS"	LJ612	25
CCCCCCCCCCCCCCCC	INPUT CARD	LJ612	26
CCCCCCCCCCCCCCCC	INPUT FOR LANE 8	LJ612	27
CCCCCCCCCCCCCCCC	VAL(I) = VALUES OF THE FIELDS 2,3,4 (FOR I=1,2,3)	LJ612	28
CCCCCCCCCCCCCCCC	OF THE "SET" INPUT CARD	LJ612	29
CCCCCCCCCCCCCCCC	INPUT FOR LANE 9	LJ612	30
CCCCCCCCCCCCCCCC	VAL(I) = VALUES OF THE FIELDS 2 THROUGH 5 (I=1 THROUGH 4)	LJ612	31
CCCCCCCCCCCCCCCC	OF THE "STG" INPUT CARD	LJ612	32
CCCCCCCCCCCCCCCC	INPUT FOR LANE 10	LJ612	33
CCCCCCCCCCCCCCCC	LO = NUMBER OF OUTPUT UNIT (PRINTER)	LJ612	34
CCCCCCCCCCCCCCCC	PRNNTC = PRINT INDICATOR	LJ612	35
CCCCCCCCCCCCCCCC	VAL(1) = SIGMA OF A CONSTITUENT, IN ANGSTROMS	LJ612	36
CCCCCCCCCCCCCCCC	VAL(2) = EPSILON/K OF A CONSTITUENT, IN KELVINS	LJ612	37
CCCCCCCCCCCCCCCC	INPUT FOR LANE 11	LJ612	38
CCCCCCCCCCCCCCCC	NOALF = INDEX OF A CONSTITUENT	LJ612	39
CCCCCCCCCCCCCCCC		LJ612	40
CCCCCCCCCCCCCCCC		LJ612	41
CCCCCCCCCCCCCCCC		LJ612	42
CCCCCCCCCCCCCCCC		LJ612	43
CCCCCCCCCCCCCCCC		LJ612	44
CCCCCCCCCCCCCCCC		LJ612	45
CCCCCCCCCCCCCCCC		LJ612	46
CCCCCCCCCCCCCCCC		LJ612	47
CCCCCCCCCCCCCCCC		LJ612	48
CCCCCCCCCCCCCCCC		LJ612	49
CCCCCCCCCCCCCCCC		LJ612	50
CCCCCCCCCCCCCCCC		LJ612	51
CCCCCCCCCCCCCCCC		LJ612	52
CCCCCCCCCCCCCCCC		LJ612	53
CCCCCCCCCCCCCCCC		LJ612	54
CCCCCCCCCCCCCCCC		LJ612	55
CCCCCCCCCCCCCCCC		LJ612	56
CCCCCCCCCCCCCCCC		LJ612	57
CCCCCCCCCCCCCCCC		LJ612	58

C	TYP(1) = SIGMA OF CONSTITUENT NOALF IN ANGSTROMS	LJ612	59
C	TYP(2) = EPSILON/K OF CONSTITUENT NOALF IN KELVINS	LJ612	60
C		LJ612	61
C	INPUT FOR LANE 12	LJ612	62
C		LJ612	63
C	LO = NUMBER OF OUTPUT UNIT (PRINTER)	LJ612	64
C	NOALF = INDEX NUMBER OF A CONSTITUENT	LJ612	65
C	PRNNTC = PRINT INDICATOR	LJ612	66
C		LJ612	67
C	INPUT FOR LANE 13	LJ612	68
C		LJ612	69
C	NOALF = INDEX NUMBER OF A CONSTITUENT	LJ612	70
C		LJ612	71
C	INPUT FOR LANE 14	LJ612	72
C		LJ612	73
C	LO = NUMBER OF OUTPUT UNIT (PRINTER)	LJ612	74
C		LJ612	75
C		LJ612	76
C	OUTPUT VARIABLES	LJ612	77
C		LJ612	78
C	OUTPUT FOR LANE 1	LJ612	79
C		LJ612	80
C	CPHI = IMPERFECTION FACTOR PHI IN THE EQUATION OF STATE	LJ612	81
C	PHIRHO = PARTIAL DERIVATIVE OF LOG(CPHI) WITH	LJ612	82
C	RESPECT TO LOG(RHU)	LJ612	83
C	PHIT = PARTIAL DERIVATIVE OF LOG(CPHI) WITH	LJ612	84
C	RESPECT TO LOG(T)	LJ612	85
C		LJ612	86
C	OUTPUT FOR LANE 2	LJ612	87
C		LJ612	88
C	INCLUDES LANE 1 OUTPUTS PLUS	LJ612	89
C	EPS = ENERGY CONTENT OF GAS DUE TO IMPERFECTION	LJ612	90
C	IN MOLES. (SEE II-C-11).	LJ612	91
C	EPSPT = PARTIAL DERIVATIVE OF (T*EPS) WITH	LJ612	92
C	RESPECT TO T, IN MOLES.	LJ612	93
C	GAMRHO(I) = PARTIAL DERIVATIVE OF GAMMA(I) WITH	LJ612	94
C	RESPECT TO LOG(RHU), I=1.....NSG.	LJ612	95
C	GAMT(I) = PARTIAL DERIVATIVE OF GAMMA(I) WITH	LJ612	96
C	RESPECT TO LOG(T), I=1.....NSG.	LJ612	97
C	PHIN(I) = PARTIAL DERIVATIVE OF LOG(CPHI) WITH	LJ612	98
C	RESPECT TO X(I), IN 1/MOLES, I=1.....NSG.	LJ612	99
C		LJ612	100
C	OUTPUT FOR LANE 3	LJ612	101
C		LJ612	102
C	GAMMA(I) = LOGARITHM OF THE ACTIVITY COEFFICIENT OF	LJ612	103
C	THE I-TH CONSTITUENT, I=1.....NSG. (SEE II-C-11)	LJ612	104
C		LJ612	105
C	OUTPUT FOR LANE 4	LJ612	106
C		LJ612	107
C	D(I,K) = PARTIAL DERIVATIVE OF GAMMA(I) WITH RESPECT	LJ612	108
C	TO X(K) IN 1/MOLES, I,K=1.....NSG. (II-C-11)	LJ612	109
C	GAMMA(I) = LOGARITHM OF THE ACTIVITY COEFFICIENT OF	LJ612	110
C	THE I-TH CONSTITUENT, I=1.....NSG.	LJ612	111
C		LJ612	112
C	OUTPUT FOR LANES 5+8 AND 11	LJ612	113
C		LJ612	114
C	NONE	LJ612	115

C		LJ612	116
C		LJ612	117
C	OUTPUT FOR LANE 6	LJ612	118
C		LJ612	119
C	NOCTS = NUMBER OF PARAMETERS THAT DEFINE THE	LJ612	120
C	EQUATION OF STATE FOR EACH CONSTITUENT.	LJ612	121
C	FOR THIS EQUATION NOCTS=2, THE TWO	LJ612	122
C	PARAMETERS ARE LENNARD-JONES POTENTIAL	LJ612	123
C	PARAMETERS SIGMA AND EPSILON/K. SEE LANE 11.	LJ612	124
C		LJ612	125
C	OUTPUT FOR LANE 7	LJ612	126
C		LJ612	127
C	KGEOS = NUMBER OF THIS EQUATION OF STATE	LJ612	128
C		LJ612	129
C	OUTPUT FOR LANE 9	LJ612	130
C		LJ612	131
C	TYP(1) = AN INDICATOR FOR SUBROUTINE LIBRARY	LJ612	132
C	ZNAME = THE VALUE OF THE NAME OF A CONSTITUENT	LJ612	133
C	VAL(3) = DEFAULT VALUE OF SIGMA	LJ612	134
C	VAL(4) = DEFAULT VALUE OF EPSILON/K	LJ612	135
C		LJ612	136
C	OUTPUT FOR LANES 10,12 AND 14	LJ612	137
C		LJ612	138
C	PRINTED OUTPUT ON UNIT LO.	LJ612	139
C		LJ612	140
C	OUTPUT FOR LANE 13	LJ612	141
C		LJ612	142
C	TYP(1) = SIGMA(NOALF) IN ANGSTROMS	LJ612	143
C	TYP(2) = EPSOK(NOALF)=EPSILON/K IN KELVINS	LJ612	144
C	(K=BOLTZMANN CONSTANT)	LJ612	145
C		LJ612	146
C	OUTPUT FOR LANE GREATER THAN 14	LJ612	147
C		LJ612	148
C	ERROR PRINT ON UNIT LO AND STOP	LJ612	149
C		LJ612	150
C	LOCAL VARIABLES	LJ612	151
C		LJ612	152
C		LJ612	153
C	ALJ61 = CODE VALUE OF THE ALPHANUMERIC NAME OF	LJ612	154
C	THIS ROUTINE "LJ612". THE VALUE IS 2624060102.0	LJ612	155
C	QZ = FACTOR B-ZERO OF THE SECOND VIRIAL COEFFICIENT	LJ612	156
C	IN (CM/ANGSTROM)**3/MOLE. SEE LANE 5.	LJ612	157
C	CKA = THIRD VIRIAL COEFFICIENT OF CONSTITUENT KA	LJ612	158
C	CZ = FACTOR C-ZERO OF THE THIRD VIRIAL COEFFICIENT	LJ612	159
C	IN (CM/ANGSTROM)**6/MOLE**2. SEE LANE 5.	LJ612	160
C	EPSAB = EPSILON/K OF THE LENNARD-JONES POTENTIAL	LJ612	161
C	BETWEEN CONSTITUENTS KA AND KB IN KELVINS.	LJ612	162
C	EPSOK(30) = ARRAY OF EPSILON/K FOR UP TO 30 CONSTITUENTS	LJ612	163
C	MISTAK = ERROR INDICATOR IN SUBROUTINE LJ612 ARGUMENTS	LJ612	164
C	NN = TEMPORARY STORAGE FOR ERROR PRINT	LJ612	165
C	RHOM = RHO/M IN 1./CM**3	LJ612	166
C	SB = WEIGHTED SUM OF B-STARS IN	LJ612	167
C	MOLES**2*ANGSTROMS**3	LJ612	168
C	SBKA(30) = PARTIAL WEIGHTED SUMS OF B-STARS IN	LJ612	169
C	MOLES*ANGSTROMS**3	LJ612	170
C	SEP = WEIGHTED SUM OF T-STAR TIMES B-STAR DERIVATIVE	LJ612	171
C	IN MOLES**2*ANGSTROM**3	LJ612	172

C	SBPKA(30) = PARTIAL WEIGHTED SUMS IN SBP	LJ612	173
C	MOLES*ANGSTROMS**3	LJ612	174
C	SB2P = WEIGHTED SUM OF (T-STAR)**2*(B-STAR-2-PRIME)	LJ612	175
C	IN MOLES**2*ANGSTROM**3	LJ612	176
C	SC = WEIGHTED SUM OF C-STARs, MOLES*ANGSTROMS**6	LJ612	177
C	SIGAB = SIGMA OF THE LENNARD-JONES 6-12 POTENTIAL	LJ612	178
C	BETWEEN CONSTITUENTS KA AND KB, ANGSTROMS	LJ612	179
C	SIGAB3 = SIGAB**3, ANGSTROMS**3	LJ612	180
C	SIGFCT = REDUCTION FACTOR OF SIGMA FOR THE RIGID SPHERE	LJ612	181
C	APPROXIMATION IN THE THIRD VIRIAL COEFFICIENT.	LJ612	182
C	DEFAULT IS 0.81	LJ612	183
C	SIGMA(30) = WELL LOCATION OF LENNARD-JONES 6-12 POTENTIAL	LJ612	184
C	(IN ANGSTROMS) FOR UP TO 30 CONSTITUENTS	LJ612	185
C	TS = T-STAR, ARGUMENT IN B-STAR TABLES	LJ612	186
C	XAB = X(KA)*X(KB) IN MOLES**2	LJ612	187
C		LJ512	188
C		LJ612	189
C		LJ612	190
C	INPUT NEEDED TO ACTIVATE THIS EQUATION OF STATE	LJ612	191
C		LJ612	192
C		LJ612	193
C	1 GEOS-INSTRUCTION SPECIFYING GASEOUS EQUATION OF STATE	LJ612	194
C	CONSISTS OF THE FOLLOWING INPUT	LJ612	195
C		LJ612	196
C	GEOS.LJ612	LJ612	197
C		LJ612	198
C	2 SET-INSTRUCTION IF THE FACTOR 0.81 FOR REDUCTION OF	LJ612	199
C	SIGMA IN THE RIGID SPHERE APPROXIMATION OF THE THIRD	LJ612	200
C	VIRIAL COEFFICIENT SHOULD BE CHANGED. SEE LINES 5 AND 8.	LJ612	201
C	THE INPUT IS AS FOLLOWS	LJ612	202
C		LJ612	203
C	SET.LJ612.SFACT.R	LJ612	204
C		LJ612	205
C	WHERE R IS THE REPLACEMENT VALUE FOR 0.81	LJ612	206
C		LJ612	207
C	3 STG-INSTRUCTIONS TO SPECIFY THE TWO PARAMETERS OF	LJ612	208
C	THE LENNARD-JONES 6-12 POTENTIAL FOR EACH	LJ612	209
C	CONSTITUENT. THE INPUTS ARE AS FOLLOWS	LJ612	210
C		LJ612	211
C	STG.LJ612.NAME.SIGMA.EOK	LJ612	212
C		LJ612	213
C	WHERE "NAME" IS THE ALPHANUMERIC NAME OF THE CONSTITUENT.	LJ612	214
C	"SIGMA" IS THE SIGMA VALUE IN ANGSTROMS (1.0E-10 METRES)	LJ612	215
C	AND "EOK" IS THE VALUE OF EPSILON/K IN KELVINS.	LJ612	216
C	K BEING THE BOLTZMANN CONSTANT 1.380662E-23 J/K	LJ612	217
C		LJ612	218
C		LJ612	219
C	AIVARS CELMINS FECIT 29 APRIL 1983.	LJ612	220
C		LJ612	221
C		LJ612	222
C	COMMON / TIGER /	LJ612	223
X	A(41,10), ADEXP, AJS(10), AJSJ, AL(40,10),	LJ612	224
X	ALPHA, AS(14,10),B(40,12), BETA, BG(30),	LJ612	225
X	IG, SJS(10), RJSJ, CC(30,12),CG(30,9),	LJ612	226
X	CHII(30), CHIJS(10),CHIJSJ, CH(25), CL(10,9),	LJ612	227
X	CN(10), CETA(10,12),CPML, CPI(30), CPJS(10),	LJ612	228
X	CPJSJ, CS(10,9), Cv, D(30,30), E,ED,	LJ612	229

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X ELM(10), EOF, EPETA1, EPETA2, EPETA3, LJ612 230
X EPETA4, EPS, EPSPS1, EPSPT, ETA(12), LJ612 231
X ETETA1(12), EO, F(30), FL, FLTA(50) LJ612 232
COMMON / TIGRE / LJ612 233
X FORM(50,20), F-EZ(40), G, GAMMA(30), GAMRHO(30), LJ612 234
X GANT(30), GETA(12), H, HCON+HO, META(12), LJ612 235
X HETAT1, HETAT2, HOF+HO, IBUG, IC(82), LJ612 236
X IDEAL, IENRON, IMIST, INOPT, INSTYP, LJ612 237
X ITCIL, ITC2L, ITC4L, ITOP, IXCC(10), LJ612 238
X IXMC(1), IXCT(10), JUMP, KGEOS, KILL, LJ612 239
X KIND(10), KPRINT, KX(30), LI, LIB, LJ612 240
X LINCT, LO+LUPT, MAXCHO, MAXFOR, MAXORD, LJ612 241
X MAXPT, MAXREJ, MIXED, NCC, NCCP, LJ612 242
COMMON / TYGER / LJ612 243
X NCC1, NCG, NCT, NCT1, NCT2, LJ612 244
X NNIS, NOALF, NOCASE, NOCHO, NOCTS, LJ612 245
X NOFLT, NOFOM, NOGC(10), NOGEOS, NOORD, LJ612 246
X NOREJ, NOTOT, NPAGE, NPTSV, NSC, LJ612 247
X NSG, NSM, NST, NTOC, ORD(25), LJ612 248
X P, PCOM, PETA(12), PETAT1, PETAT2, LJ612 249
X PHISJ(10), PHISJ, PHIN(30), PHIRHO, PHIT, LJ612 250
X PSI(30), PSIZ, PSIZZ, PO, Q(10), LJ612 251
X QA(10), R, REJ(50), RHO, RHOO, LJ612 252
COMMON / TYGRE / LJ612 253
X RS+S50, SENT+ENTE+SG(30), SQO, STOCN(10+11), LJ612 254
X STOF(11), STOGN(30+11), STOMA(11), STOMA(30), STOPC(10+11), LJ612 255
X SVOL+SVOLE+SVF(200+2), SX+50, T, TACON, TEMA(9+20), LJ612 256
X TIMITL, TMCUN, TSAVE, TYP(2), TO, LJ612 257
X UMI(30), UMJS(10), UMJSJ, V, VAL(82), LJ612 258
X VCON, VETA(12), VETAT1, VETAT2, VO, LJ612 259
X W(10), WCHI, WCP, WM, WMU, LJ612 260
X WP, WT(40), X(30), XETAT1(30), XETAT2(30), XN, LJ612 261
X XNAME(40), XUM1, XUM2, Y(30), ZC(82), ZCC(80), ZCX(80), ZNAME, LJ612 262
C LJ612 263
COMMON / PRINTC / NUPRCN, PRNNTC LJ612 264
LOGICAL PRNNTC LJ612 265
C LJ612 266
DIMENSION EPSOK(30), SIGMA(30), SSHA(30), SBPKA(30) LJ612 267
C LJ612 268
DATA ALJ612/262+060102.0/ LJ612 269
C ALJ612 IS THE REPRESENTATION OF THE ALPHANUMERIC LJ612 270
C "LJ612" IN THIS CODE. (SEE SUBROUTINE CARORD.) LJ612 271
C LJ612 272
IF(LANE.GT.14)GOTO 1500 LJ612 273
GOTO(100,100,300,400,500,600,700,800,900,1000,1100,1200, LJ612 274
+ 1300,1400),LANE LJ612 275
C LJ612 276
LANES 1 AND 2 LJ612 277
C LJ612 278
100 DO 104 KA=1,NSG LJ612 279
IF(SIGMA(KA).GT.0..AND.EPSOK(KA).GT.0.) GOTO 104 LJ612 280
C LJ612 281
101 MN=101 LJ612 282
WRITE(LO+102) MN,KA,SIGMA(KA),KA,EPSON(KA),LANE LJ612 283
102 FORMAT(10X,10X,31MENOR STOP IN EQUATION OF STATE, LJ612 284
A 29M ROUTINE LJ612 AT STATEMENT 14+9M BECAUSE//, LJ612 285
9 1M 10X,6MSIGMA(12,3M) =1PE12.5+5A.10MAND EPSON(12, LJ612 286

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C 3M(=.1PE12.5*5X*2)HARE NOT BOTH POSITIVE,/,	LJ612	287
0 1M .10X*6MLANE =.13)	LJ612	288
STOP	LJ612	289
C 104 CONTINUE	LJ612	290
C	LJ612	291
SB = 0.	LJ612	292
SBP = 0.	LJ612	293
SC = 0.	LJ612	294
SB2P = 0.	LJ612	295
C	LJ612	296
DO 145 KA=1,NSG	LJ612	297
C	LJ612	298
IF (LANE.NE.2)GOTO 105	LJ612	299
SBKA(KA)=0.	LJ612	300
SBPKA(KA)=0.	LJ612	301
C	LJ612	302
105 SC=SC+X(KA)*SIGMA(KA)**6	LJ612	303
C	LJ612	304
DO 135 KB=1,NSG	LJ612	305
C	LJ612	306
SIGAB=(SIGMA(KA)*SIGMA(KB))/2.	LJ612	307
SIGAB3=SIGAB**3	LJ612	308
EPSAB=SQRT(((SIGMA(KA)/SIGAB)*(SIGMA(KB)/SIGAB))**3	LJ612	309
*EPSOK(KA)*EPSOK(KB))	LJ612	310
XAB=X(KA)*X(KB)	LJ612	311
TS=T/EPSAB	LJ612	312
C	LJ612	313
CALL LJBS(LANE,TS*85*TBSP*TT9SPP,MISTAK)	LJ612	314
C INTERPOLATE IN THE BSTAR TABLES	LJ612	315
IF (MISTAK.EQ.0)GOTO 125	LJ612	316
111 NN=111	LJ612	317
WRITE(LO,115)NN,MISTAK,LANE,TS	LJ612	318
WRITE(LO,116)KA,KB,T	LJ612	319
STOP	LJ612	320
115 FORMAT(1M0,10X,3)HERNOR STOP IN EQUATION OF STATE.	LJ612	321
* 42H ROUTINE LJ612 AFTER CALLING INTERPOLATION.	LJ612	322
* 27H ROUTINE LJBS AT STATEMENT .14,/,	LJ612	323
*1M .10X*8M*ISTAK =.12*5X*6MLANE =.14*5X*4M*TS =.1PE12.5)	LJ612	324
116 FORMAT(1M .10X*4M*KA =.13*5X*4M*KB =.13*5X,	LJ612	325
* 3M* =.1PE12.5)	LJ612	326
C	LJ612	327
125 SB=SB+SIGAB3*85*XAB	LJ612	328
SBP=SBP+SIGAB3*TBSP*XAB	LJ612	329
IF (LANE.NE.2)GOTO 135	LJ612	330
C	LJ612	331
SBKA(KA)=SBKA(KA)+SIGAB3*85*X(KB)	LJ612	332
SBPKA(KA)=SBPKA(KA)+SIGAB3*TBSP*X(KB)	LJ612	333
SB2P=SB2P+SIGAB3*TT9SPP*XAB	LJ612	334
C	LJ612	335
135 CONTINUE	LJ612	336
C	LJ612	337
145 CONTINUE	LJ612	338
C	LJ612	339
RHOM=RH0/*M	LJ612	340
SB=BZ*SB*RHOM/5X	LJ612	341
SC=CZ*SC*RHOM**2*SA	LJ612	342
	LJ612	343

	CPHI=SB*SC-1.0	LJ612	344
	PHIRHO=(SB*2.*SC)/CPHI	LJ612	345
	SBP=9Z*SBP	LJ612	346
	PHIT=RHOM*SBP/(SX*CPHI)	LJ612	347
	IF(LANE.EQ.1) GOTO 1900	LJ612	348
C		LJ612	349
C	LANE 2	LJ612	350
C		LJ612	351
	200 EPS=-RHOM*SBP	LJ612	352
	EPSPT=-RHOM*(SBP*2.*5Z*SB20)	LJ612	353
C		LJ612	354
	DO 255 KA=1,NSG	LJ612	355
C		LJ612	356
	CKA=CZ*SIGMA(KA)**0	LJ612	357
	GAMRH0(KA)=2.*SC*2.*RHOM*HZ*SBKA(KA)*	LJ612	358
	+ (RHOM*5X)**2*CKA	LJ612	359
	GAMT(KA)=2.*RHOM*8Z*SBPKA(KA)	LJ612	360
	PHIN(KA)=(1-SB*SC)/SX*2.*RHOM*5Z*SBKA(KA)/SX	LJ612	361
	+ *RHOM*2*5X*CKA)/CPHI	LJ612	362
C		LJ612	363
	255 CONTINUE	LJ612	364
	GOTO 1900	LJ612	365
C		LJ612	366
C	LANE 3	LJ612	367
C		LJ612	368
	300 DO 305 KA=1,NSG	LJ612	369
	IF(SIGMA(KA).GT.0...AND.EPSOK(KA).GT.0.) GOTO 305	LJ612	370
C		LJ612	371
	304 NN=304	LJ612	372
	WRITE(10,102) NN,KA,SIGMA(KA),KA,EPSOK(KA),LANE	LJ612	373
	STOP	LJ612	374
C		LJ612	375
	305 CONTINUE	LJ612	376
C		LJ612	377
	SC=0	LJ612	378
	DO 345 KA=1,NSG	LJ612	379
C		LJ612	380
	SBKA(KA)=0.	LJ612	381
	GAMMA(KA)=SIGMA(KA)**6	LJ612	382
	SC=SC+GAMMA(KA)*X(KA)	LJ612	383
C		LJ612	384
	DO 335 KB=1,NSG	LJ612	385
C		LJ612	386
	SIGAB=(SIGMA(KA)+SIGMA(KB))/2.	LJ612	387
	SIGAB3=SIGAB**3	LJ612	388
	EPSAB=SQRT(1/(SIGMA(KA)/SIGAB)*(SIGMA(KB)/SIGAB))**3	LJ612	389
	+ *EPSOK(KA)*EPSOK(KB)	LJ612	390
	TS=T/EPSAB	LJ612	391
C		LJ612	392
	CALL LUBS(LANE,T,d5,TRSP,TTBSPP,MISTAK)	LJ612	393
C	INTERPOLATE IN THE BSIAK TABLES	LJ612	394
	IF(MISTAK.EQ.0) GOTO 325	LJ612	395
C		LJ612	396
	311 NN=311	LJ612	397
	WRITE(10,115) NN,MISTAK,LANE,TS	LJ612	398
	WRITE(10,116) KA,KB,T	LJ612	399
	STOP	LJ612	400

```

C STOP IF TS IS OUTSIDE THE RANGE OF THE 8STAR TABLES
C
325 SBKA(KA)=SBKA(KA)+SIGAB3*BS*X(KB)
C
335 CONTINUE
C
345 CONTINUE
C
      RHOM=RH0/WM
      DO 355 KA=1,NSG
C
      GAMMA(KA)=((GAMMA(KA)*0.5*SX*SC)+SX*RHOM*CZ+
      * 2.*SBKA(KA)*BZ)*RHOM
C GAMMA(KA) ALREADY CONTAINS C(KA)
C
355 CONTINUE
C
      GOTO 1900
C
C LANE =
C
400 SC=0
      DO 415 KA=1,NSG
C
      IF (SIGMA(KA).GT.0..AND.EPSOK(KA).GT.0.) GOTO 410
C
409 NN=409
      WRITE(LO,102) NN,KA,SIGMA(KA),KA,EPSOK(KA),LANE
      STOP
C
410 SC=SC+X(KA)*SIGMA(KA)**6
C
415 CONTINUE
C
      RHOM=RH0/WM
C
      DO 445 KA=1,NSG
C
      SBKA(KA)=0
      CKA=SIGMA(KA)**6
      GAMMA(KA)=CKA
C
      DO 435 KB=1,NSG
C
      SIGAB=(SIGMA(KA)*SIGMA(KB))/2.
      SIGAB3=SIGAB**3
      EPSAB=SQRT(((SIGMA(KA)/SIGAB)*(SIGMA(KB)/SIGAB))**3
      * *EPSOK(KA)*EPSOK(KB))
      TS=T/EPASR
C
      CALL LJB5(LANE,TS,BS,TBSP,TTBSP,M*STAK)
C INTERPOLATE IN THE 8STAR TABLES
      IF (MISTAK.EQ.0) GOTO 425
C
421 NN=421
      WRITE(LO,115) NN,MISTAK,LANE,TS
      WRITE(LO,116) KA,KB,T

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STOP	LJ612	458
C STOP IF TS IS OUTSIDE THE INTERPOLATION TABLE	LJ612	459
C	LJ612	460
425 D(KA,KB)=((SC*SA*(CKA-SIGMA(KB)**6))*CZ*RHOM	LJ612	461
*2.*BZ*BS*SIGAB3)*RHOM	LJ612	462
SBKA(KA)=SBKA(KA)*SIGAB3*BS*X(KB)	LJ612	463
C	LJ612	464
435 CONTINUE	LJ612	465
C	LJ612	466
445 CONTINUE	LJ612	467
C	LJ612	468
DO 455 KA=1,NSG	LJ612	469
GAMMA(KA)=(GAMMA(KA)*0.5*SX*SC)*SX*CZ*RHOM*	LJ612	470
A 2.*SBKA(KA)*BZ)*RHOM	LJ612	471
455 CONTINUE	LJ612	472
C	LJ612	473
GOTO 1900	LJ612	474
C	LJ612	475
LANE 5	LJ612	476
C	LJ612	477
500 BZ=1.261354	LJ612	478
SIGFCT=0.81	LJ612	479
CZ=BZ**2*(5./8.)*SIGFCT**6	LJ612	480
GOTO 1900	LJ612	481
C LANE 5 IS CALLED FROM TIGERA-10 TO ESTABLISH DEFAULT VALUES OF	LJ612	482
C CONSTANTS IN THE EQUATION OF STATE	LJ612	483
C THE SECOND VIRIAL COEFFICIENT IS B=BSTAR*BZ*SIGMA**3.	LJ612	484
C THE DIMENSION OF BZ IS (CM/ANGSTROM)**3/MOLE.	LJ612	485
C REQUIRING SIGMA IN ANGSTROM, RMO IN G/CM**3 AND	LJ612	486
C MASS MM IN GRAMS. THE VALUE OF CZ IS ACCORDING TO	LJ612	487
C MIRSCHFELDER, CURTIS AND BIRD, SECTION III-5-A, AND THE	LJ612	488
C THIRD VIRIAL COEFFICIENT IS C=CSTAR*CZ*SIGMA**6.	LJ612	489
C CZ MAY BE CHANGED IN LANE 8.	LJ612	490
C	LJ612	491
C LANE 6	LJ612	492
C	LJ612	493
600 NOCTS=2	LJ612	494
GOTO 1900	LJ612	495
C LANE 6 IS CALLED FROM TIGERA-10. NOCTS=2 INDICATES	LJ612	496
C THAT EACH CONSTITUENT IS CHARACTERIZED BY TWO	LJ612	497
C PARAMETERS WHICH SPECIFY ITS LENNARD-JONES 6-12 POTENTIAL	LJ612	498
C	LJ612	499
C LANE 7	LJ612	500
C	LJ612	501
700 IF(VAL(1).EQ.ALJ612)*GEO5=IDEAL	LJ612	502
GOTO 1900	LJ612	503
C CALLED FROM TIGERA-420 THIS INDICATES IF THE GEOS-CARD	LJ612	504
C CONTAINS THE NAME OF THIS ROUTINE:"LJ612"	LJ612	505
C	LJ612	506
C LANE 8	LJ612	507
C	LJ612	508
800 IF(VAL(1).NE.ALJ612)GOTO 1900	LJ612	509
IF(VAL(2).NE.3320151734.0)GOTO 1900	LJ612	510
SIGFCT=ABS(VAL(3))	LJ612	511
CZ=BZ**2*(5./8.)*SIGFCT**6	LJ612	512
GOTO 1900	LJ612	513
C THIS IS CALLED FROM TIGERA-440 AND IT CHANGES THE	LJ612	514

C	DEFAULT FACTOR 0.81**6=0.2824 IN THE CONSTANT C2.	LJ612	515
C	THE CODE OF VAL(2) IS "SFAC" WHICH MUST BE ON	LJ612	516
C	THE INPUT CARD AFTER "SET LJ612."	LJ612	517
C	INPUT IS THE REDUCTION FACTOR OF SIGMA AND IS RAISED TO 6-TH POWER	LJ612	518
C		LJ612	519
C	LANE 9	LJ612	520
C		LJ612	521
	900 IF(VAL(1).NE.ALJ612)GOTO 1900	LJ612	522
	TYP(1)=2.0	LJ612	523
	ZNAME=VAL(2)	LJ612	524
	IF(VAL(3).LE.0.) VAL(3) = 3.5	LJ612	525
	IF(VAL(4).LE.0.) VAL(4) = 300.	LJ612	526
	GOTO 1900	LJ612	527
C	THIS IS A CALL FROM SUBROUTINE LIBRARY-400 (III-C-245)	LJ612	528
C	PROCESSING A SIG-CARD. AT THIS TIME VAL(2) CONTAINS	LJ612	529
C	THE NAME OF THE COMPONENT. VAL(3)=SIGMA, VAL(4)=EPSOK.	LJ612	530
C	SIGMA AND EPSOK ARE REPLACED BY DEFAULT VALUES IF THEY	LJ612	531
C	ARE NOT POSITIVE.	LJ612	532
C		LJ612	533
C	LANE 10	LJ612	534
C		LJ612	535
	1000 IF(PRNNTC) WRITE(LO,1015) VAL(1)+VAL(2)	LJ612	536
	1015 FORMAT(1H ,7X,5MLJ612,3X,6MSIGMA=,1PE12.5,10H ANGSTROMS,	LJ612	537
	* 15H, EPSILON/K=,1PE12.5,8H KELVINS)	LJ612	538
	GOTO 1900	LJ612	539
C	THIS LANE IS CALLED FROM LIBRARY-940 (SEE III-C-250)	LJ612	540
C	WHICH HAS JUST STORED SIGMA AND EPSILON/K IN VAL(1) AND	LJ612	541
C	VAL(2) FOR PRINTING	LJ612	542
C		LJ612	543
C	LANE 11	LJ612	544
C		LJ612	545
	1100 SIGMA(NOALF)=TYP(1)	LJ612	546
	IF(SIGMA(NOALF).LE.0.) SIGMA(NOALF)=3.5	LJ612	547
	EPSOK(NOALF)=TYP(2)	LJ612	548
	IF(EPSOK(NOALF).LE.0.) EPSOK(NOALF)=300.	LJ612	549
	GOTO 1900	LJ612	550
C	LANE 11 IS CALLED FROM SUBROUTINE COMPOS-530 (III-C-77)	LJ612	551
C	AND SUBROUTINE RORDER-90 (III-C-312), WHICH HAVE	LJ612	552
C	STORED THE PROPER VALUES IN NOALF AND TYP. BY THIS	LJ612	553
C	CALL THE ARRAYS SIGMA AND EPSOK ARE FILLED UP AND	LJ612	554
C	REORDERED, RESPECTIVELY.	LJ612	555
C	SIGMA AND EPSOK ARE REPLACED BY THEIR DEFAULT VALUES IF	LJ612	556
C	THE VALUES IN TYP ARE NOT POSITIVE.	LJ612	557
C		LJ612	558
C	LANE 12	LJ612	559
C		LJ612	560
	1200 IF(PRNNTC) WRITE(LO,1215) SIGMA(NOALF),EPSOK(NOALF)	LJ612	561
	1215 FORMAT(1H ,13X,5MLJ612,3X,6MSIGMA=,1PE12.5,10H ANGSTROMS,	LJ612	562
	* 15H, EPSILON/K=,1PE12.5,8H KELVINS)	LJ612	563
	IF(PRNNTC.AND.SIGMA(NOALF).EQ.3.5.AND.EPSOK(NOALF).EQ.300.)	LJ612	564
	A WRITE(LO,1216)	LJ612	565
	1216 FORMAT(1H,,90X,16H(DEFAULT VALUES))	LJ612	566
	GOTO 1900	LJ612	567
C	LANE 12 IS CALLED FROM COMPOS-460 (III-C-80) WHICH	LJ612	568
C	PRINTS A LIST OF GASEOUS CONSTITUENTS	LJ612	569
C		LJ612	570
C	LANE 13	LJ612	571

C		LJ612	572
	1300 TYP(1)=SIGMA(NOALF)	LJ612	573
	TYP(2)=EPSOK(NOALF)	LJ612	574
	GOTO 1900	LJ612	575
C	THIS LANE IS CALLED FROM RORDER-40 (III-C-311) WHICH	LJ612	576
C	REORDERS THE LIST OF CONSTITUENTS. LANE 13 IS	LJ612	577
C	THE INVERSE OF LANE 11.	LJ612	578
C		LJ612	579
C	LANE 14	LJ612	580
C		LJ612	581
	1400 WRITE(LO,1415)SIGFCT	LJ612	582
	1415 FORMAT(1M0,30X,35MTRUNCATED VIRIAL EQUATION OF STATE ,	LJ612	583
	* 18M(SUBROUTINE LJ612),/.1M ,10X,	LJ612	584
	* 53MSECOND VIRIAL COEFFICIENT COMPUTED FROM LENNARD-JONES,	LJ612	585
	* 15M 6-12 POTENTIAL,/.1M 10X,	LJ612	586
	* 52MTHIRD VIRIAL COEFFICIENT COMPUTED USING A SIMPLIFIED,	LJ612	587
	* 37M RIGID SPHERE FORMULA WITH R = SIGMA*.1PE12.5)	LJ612	588
	GOTO 1900	LJ612	589
C	LANE 14 IS CALLED FROM PRINT-50 (III-C-297)REQUIRING	LJ612	590
C	TO PRINT GENERAL INFORMATION ABOUT THE EQUATION	LJ612	591
C	OF STATE	LJ612	592
C		LJ612	593
C	LANE GREATER THAN 14	LJ612	594
C		LJ612	595
	1500 WRITE(LO,1515)LANE	LJ612	596
	STOP	LJ612	597
	1515 FORMAT(1M0,10X,32MSTOP BY SUBROUTINE LJ612 BECAUSE,	LJ612	598
	* 25M IT WAS CALLED WITH LANE=.15,/.1M ,10X,	LJ612	599
	* 28MLANE SHOULD BE LESS THAN 15.)	LJ612	600
C	ERROR STOP WITH INVALID VALUE OF LANE	LJ612	601
C		LJ612	602
	1900 RETURN	LJ612	603
	END	LJ612	604

APPENDIX B
LISTING OF THE SUBROUTINE LJBS

APPENDIX B

LISTING OF THE SUBROUTINE LJBS

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SUBROUTINE LJBS(LANE,TS,BS,TBSP,TTBSP,MISTAK)
C
C THIS ROUTINE PROVIDES INTERPOLATED VALUES OF BSTAR
C AND ITS DERIVATIVES. IT IS CALLED BY THE
C TRUNCATED VIRIAL SUBROUTINE LJ612, BASED ON
C LENNARD-JONES (6-12) POTENTIAL.
C
C LANE INDICATES WHAT SHOULD BE INTERPOLATED
C   = 1 COMPUTE BSTAR AND FIRST DERIVATIVE
C   = 2 COMPUTE BSTAR AND FIRST TWO DERIVATIVES
C   = 3 COMPUTE BSTAR
C   = 4 COMPUTE BSTAR
C TS      = ARGUMENT TSTAR
C
C THE FOLLOWING WILL BE COMPUTED BY THIS ROUTINE
C
C BS      = BSTAR
C TBSP    = TSTAR*(FIRST DERIVATIVE OF BSTAR)
C TTBSP   = TSTAR**2*(SECOND DERIVATIVE OF BSTAR)
C MISTAK  = ERROR INDICATOR.
C   = 0 IF NO ERROR
C   = -1 IF TSTAR IS LESS THAN 0.01
C   = 2 IF LANE IS OUTSIDE INTERVAL (1,4)
C
C THE INTERPOLATION IS DONE IN MIRSCHFELDER-CURTIS-BIRD
C TABLES I-B USING TWO-POINT HERMITE FORMULAS IF 0.75.LE.TS.LE.5.0 .
C OUTSIDE THIS RANGE SERIES EXPANSIONS ARE USED.
C
C AIVARS CELMINS FECIT 13 APRIL 1983.
C
C   DIMENSION TRLJT(82),BSTLJ(82),BSTLJ1(82),BSTLJ2(82)
C
C THE FOLLOWING ARE MIRSCHFELDER-CURTIS-BIRD TABLES I-B
C
C   DATA (TRLJT(I),I=1,82) / .30, .35, .40, .45, .50, .55, .60, .65, .
170, .75, .80, .85, .90, .95, 1.00, 1.05, 1.10, 1.15, 1.20, 1.25, 1
2.30, 1.35, 1.40, 1.45, 1.50, 1.55, 1.60, 1.65, 1.70, 1.75, 1.80, 1
3.85, 1.90, 1.95, 2.00, 2.10, 2.20, 2.30, 2.40, 2.50, 2.6, 2.7, 2.8
4, 2.9, 3.0, 3.1, 3.2, 3.3, 3.4, 3.5, 3.6, 3.7, 3.8, 3.9, 4.0, 4.1
5 4.2, 4.3, 4.4, 4.5, 4.6, 4.7, 4.8, 4.9, 5.0, 6.0, 7.0, 8.0, 9.0
10 0.0, 20.0, 30.0, 40.0, 50.0, 60.0, 70.0, 80.0, 90.0, 100.0, 200.0
7, 300.0, 400.0/
C   DATA (BSTLJ(I),I=1,82) / -27.8805010, -18.7548950, -13.7988350, -10
1.7549750, -8.7202050, -7.2740850, -6.1979708, -5.3681918, -4.71003
270, -.41759283, -3.7342254, -3.3631193, -3.0471143, -2.7749102, -2
3.5380814, -2.3302200, -2.1463742, -1.9825492, -1.8359492, -1.70377
484, -1.5861047, -1.4752571, -1.3758479, -1.2847160, -1.2008832, -1
5.1235183, -1.0519115, -.9854534, -.9236164, -.8659428, -.8120333,
6-.7615373, -.7141473, -.6695903, -.6276254, -.5806331, -.44817100,
7-.4196776, -.3635757, -.3126134, -.2661334, -.2235863, -.1845673,
8-.1485022, -.1152339, -.0844124, -.0557670, -.0291400, -.0042809,
9.0189568, .0407201, .0611388, .0803279, .0983901, .1154169, .13149
A02, .1466837, .1610638, .1746904, .1876177, .1998951, .2115673, .2
9226751, .2332558, .2433435, .3229044, .3760885, .4134340, .4405978
C, .4608753, .5253742, .5269255, .5185750, .5083614, .4982128, .488
06507, .4797901, .4716150, .4640695, .414317, .3801279, .3583512/
C   DATA (BSTLJ1(I),I=1,82) / 76.6072560, 45.2477130, 30.2670800, 21.98

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194820, 16.9236900, 13.5821560, 11.2488490, 9.5455096, 8.2571145, 7	LJBS	59
2.2540135, 6.4541400, 5.8034061, 5.2649184, 4.8127607, 4.4282616, 4	LJBS	60
3.0976659, 3.8106421, 3.5592925, 3.3374893, 3.1404074, 2.9642040, 2	LJBS	61
4.0057826, 2.6626207, 2.5326459, 2.4141403, 2.3056683, 2.2060215, 2	LJBS	62
5.1141772, 2.0292621, 1.9505276, 1.8773287, 1.8091057, 1.7453722, 1	LJBS	63
6.6057016, 1.6297207, 1.5275444, 1.4366294, 1.3552188, 1.2819016, 1	LJBS	64
7.2155320, 1.1551691, 1.1000353, 1.0494802, 1.0029572, .9600031, .9	LJBS	65
8.202229, .8832774, .8488746, .8167606, .7867145, .7585430, .7320758	LJBS	66
9, .7071630, .6836715, .6614830, .6404922, .6206045, .6017352, .583	LJBS	67
.49082, .5667545, .5505118, .5350237, .5202387, .5061101, .4925951,	LJBS	68
.3839722, .3082566, .2524801, .2097011, .1758670, .0286638, -.0174	LJBS	69
C929, -.0393115, -.0516478, -.0593621, -.0645039, -.0680819, -.0706	LJBS	70
0470, -.0725244, -.0775400, -.0765245, -.0747534/	LJBS	71
DATA (BSTLJ2(I),I=1,82) /-356.876790, -189.465360, -116.366040, -7	LJBS	72
18.8779500, -57.3395200, -43.8924500, -34.9186900, -28.6405000, -24	LJBS	73
2.0626600, -20.6131100, -17.9419000, -15.8254600, -14.1155700, -12,	LJBS	74
37108100, -11.5398500, -10.5513300, -9.7074400, -8.9798500, -8.3470	LJBS	75
4000, -7.7921700, -7.3022700, -6.8669200, -6.4777700, -6.1280500, -	LJBS	76
55.8122500, -5.5257800, -5.2648500, -5.0262800, -4.8073800, -4.6058	LJBS	77
6700, -4.4198000, -4.2475000, -4.0875300, -3.9386300, -3.7997200, -	LJBS	78
73.5481400, -3.3264700, -3.1297400, -2.9540100, -2.7961400, -2.6535	LJBS	79
8500, -2.5241600, -2.4062300, -2.2983100, -2.1992000, -2.1078500, -	LJBS	80
92.0234000, -1.9451100, -1.8723100, -1.8044700, -1.7410800, -1.6817	LJBS	81
A400, -1.6260500, -1.5737100, -1.5244100, -1.4778900, -1.4339400, -	LJBS	82
91.3923400, -1.3529100, -1.3154800, -1.2799100, -1.2460600, -1.2138	LJBS	83
C100, -1.1830500, -1.1536700, -1.193930, -.7579300, -.6396790, -.54	LJBS	84
997929, -.4787790, -.1704030, -.0720120, -.0241090, .0039270, .0221	LJBS	85
E470, .0348170, .0440560, .0510310, .0564410, .0772960, .0813970, .	LJBS	86
F9820550/	LJBS	87
C	LJBS	88
C	LJBS	89
IF(LANE,GE,1,AND,LANE,LE,4)GOTO 15	LJBS	90
MISTAK=2	LJBS	91
RETURN	LJBS	92
C	LJBS	93
15 MISTAK=0	LJBS	94
IF(TS,GE,TRLJTB(10),AND,TS,LT,TLJTB(65)) GOTO 25	LJBS	95
IF(TS,GE,0,01) GOTO 36	LJBS	96
MISTAK=-1	LJBS	97
RETURN	LJBS	98
C	LJBS	99
C NEXT FIND SLOT FOR INTERPOLATION	LJBS	100
25 DO 35 KA=11,65	LJBS	101
IF(TS,LE,TRLJTB(KA))GOTO 45	LJBS	102
35 CONTINUE	LJBS	103
C	LJBS	104
36 CONTINUE	LJBS	105
C START COMPUTING FUNCTIONS BY SERIES EXPANSION	LJBS	106
A1=1.225 417 702 7 * SORT(2,1)*TS*(-0.25)	LJBS	107
A2=-3.625 609 908 * SORT(2,1)*0.5*TS*(-0.75)	LJBS	108
C A1 AND A2 ARE FIRST TWO TERMS OF SERIES FOR HSTAR	LJBS	109
AK=-1	LJBS	110
H5=A1+A2	LJBS	111
TBSP=(-A1-A2*3.1)/4.	LJBS	112
TTBSPP=(A1*5.-A2*21.)/16.	LJBS	113
C	LJBS	114
37 AK=AK+1.	LJBS	115

C	COMPUTE NEXT TWO TERMS OF SERIES	LJBS	116
	KVIT=1	LJBS	117
C	STOP SERIES COMPUTATION WHEN KVIT.NE.0	LJBS	118
	A1=A1*((4.0*AK-1.0)/(2.0*AK+1.0))/((2.0*AK+2.0)*TS)	LJBS	119
	A2=A2*((4.0*AK+1.0)/(2.0*AK+2.0))/((2.0*AK+3.0)*TS)	LJBS	120
	DB=A1*A2	LJBS	121
	B5=B5*DB	LJBS	122
	IF(ABS(DB).GT.1.0E-12) KVIT=0	LJBS	123
	IF(LANE.GT.2) GOTO 39	LJBS	124
C	COMPUTE ONLY BSTAR IF LANE = 3 OR 4	LJBS	125
C		LJBS	126
	DBP=-(AK+1.25)*A1-(AK+1.75)*A2	LJBS	127
	TBSP=TBSP*DBP	LJBS	128
	IF(ABS(DBP).GT.1.0E-12) KVIT=0	LJBS	129
	IF(LANE.EQ.1) GOTO 39	LJBS	130
C		LJBS	131
C	COMPUTE ALSO SECOND DERIVATIVE IF LANE = 2	LJBS	132
	DBPP=(AK+1.25)*(AK+2.25)*A1-(AK+1.75)*(AK+2.75)*A2	LJBS	133
	TBSP=TBSP*DBPP	LJBS	134
	IF(ABS(DBPP).GT.1.0E-12) KVIT=0	LJBS	135
	39 IF(KVIT.NE.0) GOTO 40	LJBS	136
C	BRANCH IF COMPUTATION CONVERGED	LJBS	137
	IF(AK.LE.305) GOTO 37	LJBS	138
C	COMPUTE AT MOST 305 TERMS OF SERIES (NEEDED FOR TS=0.01)	LJBS	139
	40 RETURN	LJBS	140
C		LJBS	141
C	ENTER 45 FROM 35 AND INTERPOLATE	LJBS	142
	45 T1=TRLJTB(KA-1)	LJBS	143
	T2=TRLJTB(KA)	LJBS	144
	DELTST=T2-T1	LJBS	145
	X1=(TS-T1)/DELTST	LJBS	146
	X2=(TS-T2)/DELTST	LJBS	147
	F1=(1.-2.*X1)*X2**2	LJBS	148
	F2=X1**2*(1.-2.*X2)	LJBS	149
	D1=X1*X2**2	LJBS	150
	D2=X1**2*X2	LJBS	151
C	F1,F2,D1,D2 ARE HERMITE INTERPOLATION FACTORS	LJBS	152
C		LJBS	153
	BS=F1*BSTLJ(KA-1)+F2*BSTLJ(KA)+	LJBS	154
	+ (D1*BSTLJ1(KA-1)+T1*D2*BSTLJ1(KA))/T2*DELTST	LJBS	155
	IF(LANE.GT.2) RETURN	LJBS	156
C	RETURN IF LANE=3 OR LANE=4	LJBS	157
C		LJBS	158
C	ELSE COMPUTE FIRST DERIVATIVE	LJBS	159
	TBSP=F1*BSTLJ1(KA-1)+F2*BSTLJ1(KA)+DELTST*	LJBS	160
	A (D1*(BSTLJ1(KA-1)+BSTLJ2(KA-1))/T1+D2*(BSTLJ1(KA)+BSTLJ2(KA))/T2)	LJBS	161
	IF(LANE.EQ.1) RETURN	LJBS	162
C		LJBS	163
C	IF LANE=2, ALSO COMPUTE SECOND DERIVATIVE	LJBS	164
	TBSP=TBSP*(BSTLJ1(KA-1)+BSTLJ1(KA))*6.*X1*X2*TS/DELTST +	LJBS	165
	A ((BSTLJ1(KA-1)+BSTLJ2(KA-1))/T1)*TS*X2*(3.*X1-1.) +	LJBS	166
	B ((BSTLJ1(KA)+BSTLJ2(KA))/T2)*TS*X1*(3.*X2-1.) - TBSP	LJBS	167
	RETURN	LJBS	168
	END	LJBS	169

APPENDIX C
SAMPLE OUTPUT

APPENDIX C

SAMPLE OUTPUT

PAGE

[illegible]

PDX SAMPLE MAY 1983 WITH LJ612 EQUATION OF STATE

PAGE 2

NAME	RDX	PERCENT BY WEIGHT	HEAT OF FORMATION (CAL/MOLE)	THE COMPOSITION IS			MOLECULAR WEIGHT	FORMULA
				STANDARD VOLUME (CC/MOLE)	STANDARD ENTROPY (CAL/K/MOLE)			
		100.00	14710.00	125.710	71.500		222.13	C ₃ H ₆ O ₆ N ₆

FOR THE COMPOSITION

THE HEAT OF FORMATION IS 66.223675 CAL/GH
 THE STANDARD VOLUME IS .565940 CC/GH
 THE STANDARD ENTROPY IS .330893 CAL/K/GH AMU
 THE STANDARD ENERGY IS 66.209969 CAL/GH.

THE ELEMENTS AND PERCENT BY MOLE

C	14.29
H	28.57
O	28.57
N	28.57

THERE ARE 11 GASEOUS CONSTITUENTS SELECTED WITH THEIR CONSTANTS

ID	NAME	STATE	STANDARD VOLUME (CC/MOLE)	STANDARD ENTROPY (CAL/K/MOLE)	HEAT OF FORMATION (CAL/MOLE)	STANDARD VOLUME (CC/MOLE)	STANDARD ENTROPY (CAL/K/MOLE)	HEAT OF FORMATION (CAL/MOLE)	STANDARD VOLUME (CC/MOLE)	STANDARD ENTROPY (CAL/K/MOLE)	HEAT OF FORMATION (CAL/MOLE)	STANDARD VOLUME (CC/MOLE)	STANDARD ENTROPY (CAL/K/MOLE)	HEAT OF FORMATION (CAL/MOLE)	STANDARD VOLUME (CC/MOLE)	STANDARD ENTROPY (CAL/K/MOLE)	HEAT OF FORMATION (CAL/MOLE)
1	1	HK	COVOLUME	40.0	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
		JK22	H	0.000	EPSILON/K	0.000											
		JK23	H	0.000	EPSILON/K	0.000											
		LJ612	SIGMA	3.50000E+00	ANGSTROMS,	.09777	-.04476	EPSILON/K=	3.00000E+02	KELVINS	-.06528	-.178910	37.8110	(DEFAULT VALUES)			
2	2	HK	COVOLUME	80.0	0.000	EPSILON/K	0.000										
		JK22	H	0.000	EPSILON/K	0.000											
		JK23	H	0.000	EPSILON/K	37.000											
		LJ612	SIGMA	2.62700E+00	ANGSTROMS,	.19299	.07446	EPSILON/K=	5.97000E+01	KELVINS	-.03514	111247.0	43.1380	(DEFAULT VALUES)			
3	3	HK	COVOLUME	140.0	0.000	EPSILON/K	0.000										
		JK22	H	0.000	EPSILON/K	0.000											
		JK23	H	0.000	EPSILON/K	0.000											
		LJ612	SIGMA	3.50000E+00	ANGSTROMS,	.21210	.02895	EPSILON/K=	3.00000E+02	KELVINS	-.00140	-1.89542	.65127	(DEFAULT VALUES)			
4	4	HK	COVOLUME	380.0	0.000	EPSILON/K	0.000										
		JK22	H	0.000	EPSILON/K	0.000											
		JK23	H	0.000	EPSILON/K	120.000											
		LJ612	SIGMA	3.00000E+00	ANGSTROMS,			EPSILON/K=	7.98000E+02	KELVINS							

RDX SAMPLE MAY 1983 WITH LJ612 EQUATION OF STATE

PAGE 2

ROX SAMPLE MAY 1983 WITH LJ612 EQUATION OF STATE

PAGE 3

THERE ARE 21 GASEOUS CONSTITUENTS SELECTED WITH THEIR CONSTANTS

5.)	MA 12	STATG	STATG	1.82197	-.44956	.03379	-4.45634	1.47414	-.17663	-18764.0	48.3899
	MA 13	HKW	CUVOLUNE	476.0	EPSILON/K	0.000					
		JC22 H	0.000	EPSILON/K	134.000						
		JC23 H	3.350	EPSILON/K	0.000						
6.)		LJ612	SIGMA=	2.90000E+00	ANGSTROMS,						
				2.25142	.04430	.00726					
		HKW	CUVOLUNE	120.0	EPSILON/K	0.000					
		JC22 H	0.000	EPSILON/K	0.000						
		JC23 H	0.000	EPSILON/K	0.000						
7.)		LJ612	SIGMA=	3.50000E+00	ANGSTROMS,						
				2.20306	1.12044	-.18445					
		HKW	CUVOLUNE	0.0	EPSILON/K	0.000					
		JC22 H	0.000	EPSILON/K	0.000						
		JC23 H	3.730	EPSILON/K	132.000						
8.)		LJ612	SIGMA=	3.46700E+00	ANGSTROMS,						
				1.53761	.06756	-.03929					
		HKW	CUVOLUNE	180.0	EPSILON/K	0.000					
		JC22 H	0.000	EPSILON/K	0.000						
		JC23 H	0.000	EPSILON/K	0.000						
9.)		LJ612	SIGMA=	3.50000E+00	ANGSTROMS,						
				5.47939	-.14543	.02109					
		HKW	CUVOLUNE	420.0	EPSILON/K	0.000					
		JC22 H	0.000	EPSILON/K	0.000						
		JC23 H	0.000	EPSILON/K	0.000						
10.)		LJ612	SIGMA=	3.50000E+00	ANGSTROMS,						
				8.97406	-.19961	.00864					
		HKW	CUVOLUNE	525.0	EPSILON/K	0.000					
		JC22 H	0.000	EPSILON/K	0.000						
		JC23 H	0.000	EPSILON/K	0.000						
11.)		LJ612	SIGMA=	3.50000E+00	ANGSTROMS,						
				3.41149	-.14971	.07777					
		HKW	CUVOLUNE	525.0	EPSILON/K	0.000					
		JC22 H	0.000	EPSILON/K	0.000						
		JC23 H	0.000	EPSILON/K	0.000						
12.)		LJ612	SIGMA=	3.50000E+00	ANGSTROMS,						
				17.83671	-.24929	.09843					
		HKW	CUVOLUNE	528.0	EPSILON/K	0.000					
		JC22 H	0.000	EPSILON/K	0.000						
		JC23 H	4.290	EPSILON/K	154.000						
		LJ612	SIGMA=	3.75800E+00	ANGSTROMS,						

ROX SAMPLE MAY 1983 WITH LJ612 EQUATION OF STATE

PAGE 3

COY SAMPLE MAY 1983 WITH L-J612 EQUATION OF STATE

TABLE I. CALCIUM COMPOUNDS SELECTED WITH THEIR CONSTANTS

[illegible]

ONLY SAMPLE MAY 1983 WITH LJA12 EVALUATION OF STATE

[illegible]

(DEF FAULT VALUES)

[illegible]

60-32611-3051C-1

```

INPUT **EXP**HUU*1.767
** ECOMP0 FHROR - STUCK IN LOCAL MINIMUM
** ECOMP0 FHROR .. STUCK IN LOCAL MINIMUM
** ECOMP0 FHROR - ETAS EXCESSIVE ITERATIONS

```

PAGE 5

THE CONSTANT VOLUME EXPLOSION STATE

TRUNCATED VIRIAL EQUATION OF STATE (SUBROUTINE LJ612)
 2-NDU VIRIAL COEFFICIENT COMPUTED FROM LENNARD-JONES 6-12 POTENTIAL
 1-THU VIRIAL COEFFICIENT COMPUTED USING A SIMPLIFIED RIGID SPHERE FORMULA WITH $\kappa = \text{SIGMA}^6 R.10000E-01$

J = ORIGINAL	V (CC/GM)	T (K)	H(O) (CAL/GM)	E(O) (CAL/GM)	S(O) (CAL/K/GM)	VUS (CC/GM)	CV (CAL/K/GM)	ALPHA	BETA	ADEXP
1.0	99541.4	4365.	1430.50	66.21	1.945	.4559	.4559	2.383	1.236	2.761

CONSTITUENT CONCENTRATIONS - MOLES PER KGW OF EXPLOSIVE

NAME	1.0
HC GAS	13.3026
H2O GAS	11.1992
CO GAS	8.9822
CU2 GAS	3.4171
H2 GAS	.7272
NH3 GAS	.3958
CH4 GAS	.0674
C2H2 GAS	.2478
C2H6 GAS	.0586
C3H8 GAS	.1142
CH3 GAS	.0484
C3H4 GAS	.0183
HI GAS	.0146
H GAS	.0020
HU GAS	.0105
CHC GAS	.0002
UE GAS	.0004
U GAS	.0001
N GAS	.0001
CH GAS	.0000
C GAS	.0000
SOLID	0.0000
TOTAL GAS	38.5570

DOX SAMPLE MAY 1983 WITH LJ612 EQUATION OF STATE

PAGE 7

INPUT "C-JIP,1,RHU,1.767

DOX SAMPLE MAY 1983 WITH LJ612 EQUATION OF STATE

PAGE 7

RDX SAMPLE MAY 1983 WITH LJA12 EQUATION OF STATE

PAGE 8

THE C-J CONDITION

THE SHOCK VELOCITY IS .6926651E+04 M/S
 THE PARTICLE VELOCITY IS .1766154E+04 M/S
 THE SOUND SPEED IS .5160498E+04 M/S
 P0 = 1.00 ATM V0 = .566 CC/GM E0 = 66.21 CAL/GM

TRUNCATED VIRIAL EQUATION OF STATE (SUBROUTINE LJA12)

SECOND VIRIAL COEFFICIENT COMPUTED FROM LENNARD-JONES 6-12 POTENTIAL
 1-JRG VIRIAL COEFFICIENT COMPUTED USING A SIMPLIFIED RIGID SPHERE FORMULA WITH $\mu = \text{SIGMA} * 8.10000E-01$
 $\mu = \text{ORIGINAL}$

P (ATM)	V (CC/GM)	T (K)	H(O) (CAL/GM)	E(O) (CAL/GM)	S(O) (CAL/K/GM)	CV (CAL/K/GM)	ALPHA	BETA	4DEXP	
1.) 21340.7	.4216	5331.	2617.43	438.99	1.916	.4216	.485	2.055	1.046	2.922

CONSTITUENT CONCENTRATIONS - MOLES PER KG OF EXPLOSIVE

NAME	1.)
HC	13.3469
H2O	10.4492
LU	5.3084
C4Z	5.9681
NH3	.1733
NH4	.1733
CH4	.5084
CH3	.5148
CH2	.5632
CH	.5823
C3H8	.0244
C3H6	.1113
CH	.0175
H	.0003
NU	.0477
CM2	.0003
U2	.0062
U	.0003
M	.0000
LM	.0001
C	.0000
50LIU	0.0000
TOTAL	36.1924

RDX SAMPLE MAY 1983 WITH LJA12 EQUATION OF STATE

PAGE 8

PDX SAMPLE MAY 1983 WITH LJO12 EQUATION OF STATE

INPUT *STUP
09.39.41.UCLP, FATH1602C:

0.966KLNS.

PAUL 9

APPENDIX D
INTERPOLATION FORMULAS

APPENDIX D

INTERPOLATION FORMULAS

In Section 6 we defined a function $B^*(T)$ by the infinite series (6.6). In order to save computing time, that function and its derivatives may be calculated by interpolation in tables instead of evaluating the series. The interpolation formulas are provided by this appendix.

The function tables in reference 2, p. 1144 ff. contain the functions $B^*, B_1^*, B_2^* = T \cdot (dB/dT)$ and $B_2^* = T^2 \cdot (d^2B/dT^2)$. Hence in addition to function values at the nodes one also has available derivatives of the functions. This permits one to use higher order two-point Hermite formulas with corresponding higher accuracy. The basic Hermite formulas are as follows. Let the function $y(x)$ and its first derivatives be given at $x = 0$ and $x = 1$, and let them be denoted by $y_0, y_1, y_0',$ and y_1' , respectively. Then an approximation to $y(x)$ is

$$h(x) = y_0 F_0(x) + y_1 F_1(x) + y_0' D_0(x) + y_1' D_1(x) \quad (D.1)$$

The error of the approximation is of fourth order in x . The derivative of (D.1) is an approximation of $y'(x)$ with a third order error:

$$h'(x) = y_0 F_0'(x) + y_1 F_1'(x) + y_0' D_0'(x) + y_1' D_1'(x) \quad (D.2)$$

The Hermite factors in Eqs. (D.1) and (D.2) are

$$\begin{aligned} F_0(x) &= (x-1)^2 (1+2x) \\ F_1(x) &= x^2 (1-2(x-1)) \\ D_0(x) &= (x-1)^2 x \\ D_1(x) &= x^2 (x-1) \\ F_0'(x) &= 6x(x-1) \\ F_1'(x) &= -6x(x-1) \\ D_0'(x) &= (x-1)(3x-1) \\ D_1'(x) &= x(3(x-1)+1) \end{aligned} \quad (D.3)$$

For an interpolation in the $\bar{T}$ -table between $\bar{T}_a$ and $\bar{T}_b$ one has the definition

$$x = (\bar{T} - \bar{T}_a) / (\bar{T}_b - \bar{T}_a) \quad , \quad (D.4)$$

and derivatives are transformed by using the chain rule

$$\frac{d}{dx} = (\bar{T}_b - \bar{T}_a) \frac{d}{d\bar{T}} \quad . \quad (D.5)$$

Hence $\bar{B}$ may be interpolated by the formula

$$\bar{B} = \bar{B}_a F_0 + \bar{B}_b F_1 + (\bar{T}_b - \bar{T}_a) \left(\frac{\bar{B}_{1a}}{\bar{T}_a} D_0 + \frac{\bar{B}_{1b}}{\bar{T}_b} D_1 \right) \quad . \quad (D.6)$$

In order to compute $\bar{B}_1 = \bar{T} \bar{B}'$ one can either interpolate $\bar{B}'$ making use of the relation $\bar{B}'' = \bar{B}_2 / \bar{T}$ or interpolate the function $\bar{B}_1$ itself, or compute the derivative of Eq. (D.6), thereby disregarding the $\bar{B}_2$ tables. It was found from numerical experiments (by comparing interpolated values with exact values) that the first approach is not very accurate. The third approach cannot be recommended in general and, therefore, it was not tried. The final algorithm was based on the second approach and implemented as follows. The derivative of the function $\bar{B}_1$ is given the terms of $\bar{B}_1$ and $\bar{B}_2$ by the formula

$$\frac{d}{d\bar{T}} \bar{B}_1 = \frac{d}{d\bar{T}} (\bar{T} \bar{B}') = \frac{1}{\bar{T}} (\bar{T} \bar{B}' + \bar{T}^2 \bar{B}'') = \frac{1}{\bar{T}} (\bar{B}_1 + \bar{B}_2) \quad . \quad (D.7)$$

Using this value in the interpolation formula (D.1) one obtains

$$\bar{B}_1 = \bar{B}_{1a} F_0 + \bar{B}_{1b} F_1 + (\bar{T}_b - \bar{T}_a) \left[\frac{\bar{B}_{1a} + \bar{B}_{2a}}{\bar{T}_a} D_0 + \frac{\bar{B}_{1b} + \bar{B}_{2b}}{\bar{T}_b} D_1 \right] \quad . \quad (D.8)$$

The function $\bar{B}_2$ was interpolated by using the inversion of Eq. (D.7):

$$\bar{B}_2 = \bar{T} \bar{B}'_1 - \bar{B}_1 = \frac{\bar{T}}{\bar{T}_b - \bar{T}_a} \frac{d\bar{B}_1}{dx} - \bar{B}_1 \quad . \quad (D.9)$$

In this formula the x -derivative was computed by differentiation of Eq. (D.8), that is, by Eq. (D.2). After substitution and simple manipulation one obtains

$$\bar{B}_2 = \bar{T} \left[\frac{\bar{B}_{1b} - \bar{B}_{1a}}{\bar{T}_b - \bar{T}_a} F'_1 + \frac{\bar{B}_{1a} + \bar{B}_{2a}}{\bar{T}_a} D'_0 + \frac{\bar{B}_{2b} + \bar{B}_{2a}}{\bar{T}_b} D'_1 \right] - \bar{B}_1, \quad (D.10)$$

where the relation $F'_0 = -F'_1$ has been used.

Limited comparison of the interpolation results with exact values showed reasonable agreement (eight digits for $\bar{B}$, four digits for $\bar{B}_2$). The routine LJBS can easily be changed to produce exact function values for all $\bar{T}$ by series evaluation instead of interpolation. The corresponding increase of computing time was found to be less than two percent.

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