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# A VIRIAL EQUATION OF STATE OPTION FOR THE TIGER COMPUTER PROGRAM

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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

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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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## 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 for 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:

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

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

with

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

In these equations, p (Pa) is the pressure, R = 8.3143 J/(K·mol) is the universal gas constant, T (K) is temperature, $\tilde{V}$ ($m^3$/mol) is the molar volume, $\phi$ 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 $\phi$ 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

$$\phi(r) = 4\,\varepsilon\,[(\sigma/r)^{12} - (\sigma/r)^6] \tag{2.3}$$

where r (m) is the distance between molecules, and $\varepsilon$ (J) and $\sigma$ (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. $\sigma$ is that value of r for which $\phi(r) = 0$, and $\varepsilon$ 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 $\sigma$ are around $3.5 \cdot 10^{-10}$ m. The parameter $\varepsilon$ enters the present calculations only in the ratio $\varepsilon/k$, where $k = 1.38054 \cdot 10^{-22}$ J/K is the Boltzmann constant. Typical values of the ratio $\varepsilon/k$ are around 300 K.

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

$$\overset{*}{T} = T\,k/\varepsilon \tag{2.4}$$

and a reduced dimensionless coefficient $\overset{*}{B}$ by

$$\overset{*}{B} = B/b_o(\sigma) \tag{2.5}$$

where

---

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

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

and $\tilde{N} = 6.02252 \cdot 10^{23}$ $mol^{-1}$ is the Avogadro number. $\overset{*}{B}$ is for a given intermolecular potential function of Lennard-Jones type a unique function of $\overset{*}{T}$. 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, $\sigma$ and $\varepsilon$ is in terms of the function $\overset{*}{B}$ as follows

$$B(T) = b_o(\sigma) \cdot \overset{*}{B}(T\ k/\varepsilon) \quad . \tag{2.7}$$

For gas mixtures the computation of B(T) is modified such that in Eq. (2.7) one uses for $\sigma$ and $\varepsilon$ 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:

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

where $b_o(\sigma)$ 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.

---

[3] *E. 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 $\sigma$ and $\varepsilon$ 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:

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

$$\varepsilon/k = 300 \text{ K} \quad . \tag{2.9}$$

## 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 $\sigma$ and $\varepsilon/k$ are provided by a STG-card for each gaseous contituent. 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,σ, ε/k
```

Other STG-cards specifying constants for the BKW, JCZ2 or JCZ3 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 $\sigma$ must be entered in $10^{-10}$ m (in ångströms) and the value of $\varepsilon/k$ 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 $\varepsilon/k = 542.5$ K. If either $\sigma$ or $\varepsilon/k$ is negative or zero in the STG-card, then the corresponding default value ($\sigma = 3.5 \cdot 10^{-10}$ m, $\varepsilon/k = 300$ 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

$$p = \frac{RT}{\tilde{V}} \Phi(\tilde{V},T) \tag{5.1}$$

where

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

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):

$$\tilde{V} = \frac{1}{n} V = \frac{1}{n} \frac{M_g}{\rho} = \frac{1}{n} \frac{M_o}{\hat{\rho}} \tag{5.3}$$

where n is the number of moles, V is the gas volume, $M_g$ is the mass of the gas, $\rho$ 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, ..., s. Then

$$n = \sum_{i=1}^{s} n_i \quad . \tag{5.4}$$

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

$$p = R\,T\,n\,\frac{\hat{\rho}}{M_o}\,\Phi \tag{5.5}$$

with

$$\begin{aligned}\Phi &= \Phi(\hat{\rho}, T, M_o, n_1, n_2, \ldots, n_s) \\ &= 1 + \frac{\hat{\rho}}{M_o}\,n\,B(T,n_1, \ldots,n_s) + \left(\frac{\hat{\rho}}{M_o}\right)^2 n^2\,C(n_1, \ldots, n_s) \quad .\end{aligned} \tag{5.6}$$

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 $\sigma_i$ and $\varepsilon_i$, 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)

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

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

$$B_{ij} = B_{ij}(T,\sigma_i,\sigma_j,\varepsilon_i/k,\varepsilon_j/k) \quad , \tag{5.8}$$

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

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

of the third virial coeffients $C_i$ of the individual constituents. The latter are assumed to be independent of temperature and $\varepsilon_i$, that is,

$$C_i = C_i(\sigma_i) \quad . \tag{5.10}$$

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

In order to simplify the following formulas, we define

$$\sum_B = \sum_{i=1}^{s} \sum_{j=1}^{s} n_i n_i B_{ij} \quad , \tag{5.11}$$

$$\sum_B' = \sum_{i=1}^{s} \sum_{i=j}^{s} n_i n_j \frac{dB_{ij}}{dT} \quad , \tag{5.12}$$

$$\sum_B'' = \sum_{i=1}^{s} \sum_{j=1}^{s} n_i n_j \frac{d^2 B_{ij}}{dT^2} \tag{5.13}$$

and

$$\sum_C = \sum_{i=1}^{s} n_i C_i \quad . \tag{5.14}$$

The imperfection parameter $\Phi$ is given in terms of these quantities by

$$\Phi = 1 + \frac{\hat{\rho}}{M_o} \frac{1}{n} \sum_B + \left(\frac{\hat{\rho}}{M_o}\right)^2 n \sum_C \quad . \tag{5.15}$$

The TIGER program carries out a number of different computations for which it needs in addition to the value of the imperfection parameter $\Phi$ also the values of certain expressions involving $\Phi$. 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 $\Phi$:

$$\frac{\partial \ln \Phi}{\partial \ln \hat{\rho}} = \frac{\hat{\rho}}{\Phi} \frac{\partial \Phi}{\partial \hat{\rho}} = \frac{1}{\Phi} \left(\frac{\hat{\rho}}{M_o} \frac{1}{n} \sum_B + 2\left(\frac{\hat{\rho}}{M_o}\right)^2 n \sum_C\right) \quad , \tag{5.16}$$

$$\frac{\partial \ln \Phi}{\partial \ln T} = \frac{T}{\Phi} \frac{\partial \Phi}{\partial T} = \frac{1}{\Phi} \frac{\hat{\rho}}{M_o} \frac{1}{n} T \sum_B' \tag{5.17}$$

and

$$\frac{\partial \ln \phi}{\partial n_i} = \frac{1}{\phi}\frac{\partial \phi}{\partial n_i} = \frac{1}{\phi}\left\{\frac{1}{n}\left[-\frac{\hat{\rho}}{M_o}\frac{1}{n}\sum_B + \left(\frac{\hat{\rho}}{M_o}\right)^2 n \sum_C\right] + \right.$$

$$\left. + \frac{\hat{\rho}}{M_o}\frac{2}{n}\sum_{j=1}^{s} n_j B_{ij} + \left(\frac{\hat{\rho}}{M_o}\right)^2 n\, C_i\right\} \quad . \tag{5.18}$$

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

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

$$= \int_0^{\hat{\rho}} \left[\phi - 1 + n\frac{\partial \phi}{\partial n_i}\right]\frac{d\hat{\rho}}{\hat{\rho}} \quad . \tag{5.19}$$

An evaluation of the integral (5.19) yields for $\Gamma_i$ the formula

$$\Gamma_i = 2\frac{\hat{\rho}}{M_o}\sum_{j=1}^{s} n_j B_{ij} + \frac{1}{2}\left(\frac{\hat{\rho}}{M_o}\right)^2 n^2 C_i + \left(\frac{\hat{\rho}}{M_o}\right)^2 n \sum_C \quad . \tag{5.20}$$

Other expressions needed by the TIGER program are the following two dimensionless derivatives of $\Gamma_i$:

$$\frac{\partial \Gamma_i}{\partial \ln \hat{\rho}} = \hat{\rho}\frac{\partial \Gamma_i}{\partial \hat{\rho}} = 2\frac{\hat{\rho}}{M_o}\sum_{j=1}^{s} n_j B_{ij} + \left(\frac{\hat{\rho}}{M_o}\right)^2 n^2 C_i + 2\left(\frac{\hat{\rho}}{M_o}\right)^2 n \sum_C \tag{5.21}$$

and

$$\frac{\partial \Gamma_i}{\partial \ln T} = T\frac{\partial \Gamma_i}{\partial T} = 2\frac{\hat{\rho}}{M_o}\sum_{j=1}^{s} n_j T\frac{dB_{ij}}{dT} \quad , \tag{5.22}$$

and the following derivative with the dimension 1/mol

$$\frac{\partial \Gamma_i}{\partial n_j} - 2\frac{\hat{\rho}}{M_o} B_{ij} + \left(\frac{\hat{\rho}}{M_o}\right)^2\left[\sum_C + n\,(C_i + C_j)\right] \quad . \tag{5.23}$$

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

$$\varepsilon = \int_0^{\hat{\rho}} \frac{M_o}{R\,T\,\hat{\rho}} \left(p - T\frac{\partial p}{\partial T}\right) \frac{d\hat{\rho}}{\hat{\rho}} = -\int_0^{\hat{\rho}} T\,\frac{\partial(n\phi)}{\partial T}\,\frac{d\hat{\rho}}{\hat{\rho}} \tag{5.24}$$

and

$$\varepsilon_T' = -\int_0^{\hat{\rho}} \frac{M_o T}{R\,\hat{\rho}}\,\frac{\partial^2 p}{\partial T^2}\,\frac{d\hat{\rho}}{\hat{\rho}} = \frac{\partial(T\varepsilon)}{\partial T} \quad . \tag{5.25}$$

An evaluation of these expressions yields

$$\varepsilon = \frac{\hat{\rho}}{M_o}\,T\,\underset{\sim}{\Gamma}_B' \tag{5.26}$$

and

$$\varepsilon_T' = -\frac{\hat{\rho}}{M_o}\left(2\,T\,\underset{\sim}{\Gamma}_B' + T^2\,\underset{\sim}{\Gamma}_B''\right) \quad . \tag{5.27}$$

We notice that the quantity $\varepsilon$ 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 $\varepsilon$.

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 $T^2 \cdot d^2B_{ij}/dT^2$, 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 $\sigma_{ij}$ and $\varepsilon_{ij}$ of the mixture potential (Ref. 2, p. 168, Ref. 3, p. 11):

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

and

$$\frac{\varepsilon_{ij}}{k} = \left(\frac{\sigma_i}{\sigma_{ij}} \cdot \frac{\sigma_j}{\sigma_{ij}}\right)^{3/2} \left(\frac{\varepsilon_i}{k} \cdot \frac{\varepsilon_j}{k}\right)^{1/2} \quad . \tag{6.2}$$

We notice that for $i=j$ these formulas produce $\sigma_{ii} = \sigma_i$, $\varepsilon_{ii} = \varepsilon_i$ and, consequently, $B_{ii} = B_i$. The $\sigma_{ij}$ and $\varepsilon_{ij}$ 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 $\overset{*}{T}$ and computing a corresponding dimensionless virial coefficient $\overset{*}{B}(\overset{*}{T})$ from which $B_{ij}$ then can be retrieved. The function $\overset{*}{B}(\overset{*}{T})$ is uniquely determined by the constants of the Lennard-Jones potential. The following formulas are used to carry out this calculation:

$$\overset{*}{T} = T\, k/\varepsilon_{ij} \quad , \tag{6.3}$$

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

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

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

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

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

with

$$b_m = -\frac{2^m \sqrt{2}}{4 \cdot m!}\, \Gamma\left(-\frac{1}{4} + \frac{1}{2} m\right) \quad . \tag{6.7}$$

The first two coefficients in the series (6.6) are[4]

[4] *P. Jahnke and F. Emde, "Tables of Higher Functions," B.G. Teubner, Leipzig 1948.*

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

and

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

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

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

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

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

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

$$A_{0,0} = b_0\, \overset{*}{T}^{\,(-1/4)} \quad , \tag{6.12}$$

$$A_{1,0} = b_1\, \overset{*}{T}^{\,(-3/4)} \tag{6.13}$$

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

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

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

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

$$\overset{*}{T}\frac{d\overset{*}{B}}{d\overset{*}{T}} = \sum_{m=0}^{\infty}\left(-\frac{4m+1}{4}A_{0,m} - \frac{4m+3}{4}A_{1,m}\right) \tag{6.16}$$

and

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

The evaluation of the series (6.11), (6.16) and (6.17) is done in the subroutine LJBS which computes for given $\overset{*}{T}$ the corresponding values of $\overset{*}{B}$, $\overset{*}{T}\overset{*}{B}'$ and $\overset{*}{T}^2\overset{*}{B}''$. The series converge very fast if $\overset{*}{T}$ is large, but require the computation of a large number of terms if $\overset{*}{T}$ is small. Typical TIGER computations are done with values of $\overset{*}{T}$ between one and two. In that range some computation time can be saved by interpolating $\overset{*}{B}(\overset{*}{T})$ 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 $\overset{*}{B}$ and its derivatives by interpolation if $\overset{*}{T}$ is within the range (0.75, 5.0). If $\overset{*}{T} = 5.0$, then only six to seven terms of the series have to be calculated, and the number of terms decreases as $\overset{*}{T}$ 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 $\overset{*}{T} < 0.75$ 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 $\overset{*}{T} = 0.01$. However, one would not expect typical TIGER calculations to be done for $\overset{*}{T} < 0.75$. For $\overset{*}{T} < 0.01$ 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

$$C_i = \frac{5}{8} \cdot \left(\frac{2}{3} \pi \tilde{N}\right)^2 \cdot (0.81 \cdot \sigma_i)^6 \qquad (7.1)$$

where $\tilde{N} = 6.02252 \cdot 10^{23}$ $mol^{-1}$ is the Avogadro constant and $\sigma_i$ 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 $\overset{*}{T} \approx 60$. (See Eqs. (2.4) and (6.3) for the definition of the reduced temperature $\overset{*}{T}$.) Theoretically the factor may be increased to about 0.99 for $\overset{*}{T} = 1.25$ (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 $\overset{*}{B}$ and its derivatives for given $\overset{*}{T}$. The latter is a reduced dimensionless temperature and $\overset{*}{B}$ 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 ($\partial(\ln \phi)/\partial n_i$, $\partial \Gamma_j/\partial n_i$, $\varepsilon$, $\varepsilon'_T$) 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 $\sigma$ and kelvins for $\varepsilon/k$. 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

```
      SUBROUTINE LJ612(LANE)
C
C     PURPOSE
C
C       TO COMPUTE THE OUTPUT FOR STATEG USING A TRUNCATED
C       VIRIAL EQUATION OF STATE IN WHICH THE SECOND COEFFICIENT
C       IS BASED ON LENNARD-JONES 6-12 POTENTIAL AND
C       THE THIRD COEFFICIENT IS COMPUTED USING A
C       SIMPLIFIED RIGID SPHERE FORMULA
C
C       INPUT AND OUTPUT DEPEND ON THE VALUE OF LANE
C
C           INPUT VARIABLES
C
C     INPUT FOR LANES 1 THROUGH 4
C
C       LO          = NUMBER OF OUTPUT UNIT (PRINTER)
C       NSG         = NUMBER OF GASEOUS CONSTITUENTS
C       RHO         = MASS OF MIXTURE PER VOLUME OF GAS IN G/CM**3
C                     THIS IS CALLED RHO-HAT IN TEXT, SEE I-B-16.
C       SX          = SUM OF GASEOUS MOLE NUMBERS X(I), IN MOLES.
C       T           = GAS TEMPERATURE IN KELVINS
C       WM          = REFERENCE MASS IN GRAMS (M-ZERO IN I-B-16)
C       X(I)        = MOLE NUMBER OF THE I-TH GASEOUS CONSTITUENT
C                     WITH I=1,...., NSG, IN MOLES
C
C     INPUT FOR LANES 5 AND 6
C
C       NONE
C
C     INPUT FOR LANE 7
C
C       IDEAL       = NUMBER OF THIS EQUATION OF STATE
C       VAL(1)      = VALUE OF THE SECOND FIELD OF THE "GEOS"
C                     INPUT CARD
C
C     INPUT FOR LANE 8
C
C       VAL(I)      = VALUES OF THE FIELDS 2,3,4 (FOR I=1,2,3)
C                     OF THE "SET" INPUT CARD
C
C     INPUT FOR LANE 9
C
C       VAL(I)      = VALUES OF THE FIELDS 2 THROUGH 5 (I=1 THROUGH 4)
C                     OF THE "STG" INPUT CARD
C
C
C     INPUT FOR LANE 10
C
C       LO          = NUMBER OF OUTPUT UNIT (PRINTER)
C       PRNNTC      = PRINT IDICATOR
C       VAL(1)      = SIGMA OF A CONSTITUENT, IN ANGSTROMS
C       VAL(2)      = EPSILON/K OF A CONSTITUENT, IN KELVINS
C
C     INPUT FOR LANE 11
C
C       NOALF       = INDEX OF A CONSTITUENT
```

```
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(RHO)                                    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(RHO).  I=1,...,NSG.                     LJ612    95
C        GAMT(I)    = PARTIAL DERIVATIVE OF GAMMA(I) WITH                    LJ612    96
C                     RESPECT TO LOG(T).  I=1,...,NGG.                       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     OUTPUT FOR LANE 6                                                 LJ612   117
C                                                                       LJ612   118
C       NOCTS      = NUMBER OF PARAMETERS THAT DEFINE THE               LJ612   119
C                    EQUATION OF STATE FOR EACH CONSTITUENT.            LJ612   120
C                    FOR THIS EQUATION NOCTS=2, THE TWO                 LJ612   121
C                    PARAMETERS ARE LENNARD-JONES POTENTIAL             LJ612   122
C                    PARAMETERS SIGMA AND EPSILON/K. SEE LANE 11.       LJ612   123
C                                                                       LJ612   124
C     OUTPUT FOR LANE 7                                                 LJ612   125
C                                                                       LJ612   126
C       KGEOS      = NUMBER OF THIS EQUATION OF STATE                   LJ612   127
C                                                                       LJ612   128
C     OUTPUT FOR LANE 9                                                 LJ612   129
C                                                                       LJ612   130
C       TYP(1)     = AN INDICATOR FOR SUBROUTINE LIBRARY                LJ612   131
C       ZNAME      = THE VALUE OF THE NAME OF A CONSTITUENT             LJ612   132
C       VAL(3)     = DEFAULT VALUE OF SIGMA                             LJ612   133
C       VAL(4)     = DEFAULT VALUE OF EPSILON/K                         LJ612   134
C                                                                       LJ612   135
C     OUTPUT FOR LANES 10,12 AND 14                                     LJ612   136
C                                                                       LJ612   137
C       PRINTED OUTPUT ON UNIT LO.                                      LJ612   138
C                                                                       LJ612   139
C     OUTPUT FOR LANE 13                                                LJ612   140
C                                                                       LJ612   141
C       TYP(1)     = SIGMA(NOALF) IN ANGSTROMS                          LJ612   142
C       TYP(2)     = EPSOK(NOALF)=EPSILON/K IN KELVINS                  LJ612   143
C                    (K=BOLTZMANN CONSTANT)                             LJ612   144
C                                                                       LJ612   145
C     OUTPUT FOR LANE GREATER THAN 14                                   LJ612   146
C                                                                       LJ612   147
C       ERROR PRINT ON UNIT LO AND STOP                                 LJ612   148
C                                                                       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       BZ         = 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 LJBS ARGUMENTS       LJ612   164
C       NN         = TEMPORARY STORAGE FOR ERROR PRINT                  LJ612   165
C       RHOM       = RHO/GM 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       SBP        = WEIGHTED SUM OF T-STAR TIMES B-STAR DERIVATIVE     LJ612   171
C                    IN MOLES**2*ANGSTROM**3                            LJ612   172
```

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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 OS 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                                                                       LJ612    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 LANES 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
      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    BIG,      BJS(10),  BJSJ,     CC(30,12),CG(30,9),            LJ612    226
     X    CHII(30), CHIJS(10),CHIJSJ,   CHO(25),  CL(10,9),            LJ612    227
     X    CN(10),   CNETA(10,12),CPHI,  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,      EPSPSI,   EPSPT,    ETA(12),               LJ612    231
     X    ETETA1(12),E0,      F(30),    FL,       FLTA(50)               LJ612    232
      COMMON / TIGRE /                                                   LJ612    233
     X    FORM(50,20),FREZ(40),G,       GAMMA(30),GAMRHO(30),          LJ612    234
     X    GAMT(30), GETA(12), H,        HCON,HD,  HETA(12),              LJ612    235
     X    HETAT1,   HETAT2,   HOF,HO,   IBUG,     IC(82),                LJ612    236
     X    IDEAL,    IERROR,   IHIST,    INOPT,    INSTYP,                LJ612    237
     X    ITC1L,    ITC2L,    ITC4L,    ITOP,     IXCC(10),              LJ612    238
     X    IXMC(10), IXCT(10), JUMP,     KGEOS,    KILL,                  LJ612    239
     X    KIND(10), KPRINT,   KX(30),   LI,       LIB,                   LJ612    240
     X    LINCT,    LO,LOPT,  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,    NOFORM,   NOGC(10), NOGEOS,   NGORD,                 LJ612    246
     X    NOREJ,    NOTOT,    NPAGE,    NPTSV,    NSC,                   LJ612    247
     X    NSG,      NSM,      NST,      NTOC,     ORD(25),               LJ612    248
     X    P,        PCON,     PETA(12), PETAT1,   PETAT2,                LJ612    249
     X    PHIJS(10),PHIJSJ,   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    RX,S,SD,  SENT,SENTE,SG(30),  SQQ,      STOCN(10,11),          LJ612    254
     X    STOFL(11),STOGN(30,11),STOMA(11),STONA(30),STOPC(10,11),       LJ612    255
     X    SVOL,SVOLE,SVP(200,2),SX,SO,  T,        TACON, TEMA(9,20),     LJ612    256
     X    TINITL,   TMCON,    TSAVE,    TYP(82),  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 / NOPRCN,PRNNTC                                    LJ612    264
      LOGICAL PRNNTC                                                     LJ612    265
C                                                                        LJ612    266
      DIMENSION EPSOK(30),SIGMA(30),SBRKA(30),SBPKA(30)                  LJ612    267
C                                                                        LJ612    268
      DATA ALJ612/2624060102.0/                                          LJ612    269
C  ALJ612 IS THE REPRESENTATION OF THE ALPHANUMERIC                      LJ612    270
C  "LJ612" IN THIS CODE. (SEE SUBROUTINE CARDRD.)                        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
C  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 NN=101                                                             LJ612    282
      WRITE(LO,102) NN,KA,SIGMA(KA),KA,EPSOK(KA),LANE                    LJ612    283
  102 FORMAT(1H0,10X,31HERROR STOP IN EQUATION OF STATE,                 LJ612    284
     A 29H ROUTINE LJ612 AT STATEMENT ,I4,9H  BECAUSE,/,                 LJ612    285
     B 1H ,10X,6HSIGMA(,I2,3H) =,1PE12.5,5X,10HAND EPSOK(,I2,            LJ612    286
```

```
      C 3H( =,1PE12.5,5X,21HARE NOT BOTH POSITIVE,/,                    LJ612    287
      D 1H ,10X,6HLANE =,I3)                                            LJ612    288
       STOP                                                             LJ612    289
C                                                                       LJ612    290
  104 CONTINUE                                                          LJ612    291
C                                                                       LJ612    292
       SB = 0.                                                          LJ612    293
       SBP= 0.                                                          LJ612    294
       SC  =  0.                                                        LJ612    295
       SB2P= 0.                                                         LJ612    296
C                                                                       LJ612    297
       DO 145 KA=1,NSG                                                  LJ612    298
C                                                                       LJ612    299
       IF(LANE.NE.2)GOTO 105                                            LJ612    300
       SBKA(KA)=0.                                                      LJ612    301
       SBPKA(KA)=0.                                                     LJ612    302
C                                                                       LJ612    303
  105 SC=SC+X(KA)*SIGMA(KA)**6                                          LJ612    304
C                                                                       LJ612    305
       DO 135 KB=1,NSG                                                  LJ612    306
C                                                                       LJ612    307
       SIGAB=(SIGMA(KA)+SIGMA(KB))/2.                                   LJ612    308
       SIGAB3=SIGAB**3                                                  LJ612    309
       EPSAB=SQRT(((SIGMA(KA)/SIGAB)*(SIGMA(KB)/SIGAB))**3              LJ612    310
     + *EPSOK(KA)*EPSOK(KB))                                            LJ612    311
       XAB=X(KA)*X(KB)                                                  LJ612    312
       TS=T/EPSAB                                                       LJ612    313
C                                                                       LJ612    314
       CALL LJBS(LANE,TS,BS,TBSP,TTBSPP,MISTAK)                         LJ612    315
C  INTERPOLATE IN THE BSTAR TABLES                                      LJ612    316
       IF(MISTAK.EQ.0)GOTO 125                                          LJ612    317
  111 NN=111                                                            LJ612    318
       WRITE(LO,115)NN,MISTAK,LANE,TS                                   LJ612    319
       WRITE(LO,116)KA,KB,T                                             LJ612    320
       STOP                                                             LJ612    321
  115 FORMAT(1H0,10X,31HERROR STOP IN EQUATION OF STATE,                LJ612    322
     + 42H ROUTINE LJ612 AFTER CALLING INTERPOLATION,                   LJ612    323
     + 27H ROUTINE LJBS AT STATEMENT ,I4,/,                             LJ612    324
     +1H ,10X,8HMISTAK =,I2,5X,6HLANE =,I4,5X,4HTS =,1PE12.5)           LJ612    325
  116 FORMAT(1H ,10X,4HKA =,I3,5X,4HKB =,I3,5X,                         LJ612    326
     + 3HT =,1PE12.5)                                                   LJ612    327
C                                                                       LJ612    328
  125 SB=SB+SIGAB3*BS*XAB                                               LJ612    329
       SBP=SBP+SIGAB3*TBSP*XAB                                          LJ612    330
       IF(LANE.NE.2)GOTO 135                                            LJ612    331
C                                                                       LJ612    332
       SBKA(KA)=SBKA(KA)+SIGAB3*BS*X(KB)                                LJ612    333
       SBPKA(KA)=SBPKA(KA)+SIGAB3*TBSP*X(KB)                            LJ612    334
       SB2P=SB2P+SIGAB3*TTBSPP*XAB                                      LJ612    335
C                                                                       LJ612    336
  135 CONTINUE                                                          LJ612    337
C                                                                       LJ612    338
  145 CONTINUE                                                          LJ612    339
C                                                                       LJ612    340
       RHOM=RHO/SM                                                      LJ612    341
       SB=BZ*SB*RHOM/SX                                                 LJ612    342
       SC=CZ*SC*RHOM**2*SX                                              LJ612    343
```

```
      CPMI=SB+SC+1.0                                                    LJ612    344
      PMIRHO=(SB+2.*SC)/CPMI                                            LJ612    345
      SBP=BZ*SBP                                                        LJ612    346
      PMIT=RHOM*SBP/(SX*CPMI)                                           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.+BZ*SB2P)                                      LJ612    353
C                                                                       LJ612    354
      DO 255 KA=1,NSG                                                   LJ612    355
C                                                                       LJ612    356
      CKA=CZ*SIGMA(KA)**6                                               LJ612    357
      GAMRHO(KA)=2.*SC+2.*RHOM*BZ*SBKA(KA)+                             LJ612    358
     + (RHOM*SX)**2*CKA                                                 LJ612    359
      GAMT(KA)=2.*RHOM*BZ*SBPKA(KA)                                     LJ612    360
      PMIN(KA)=((-SB+SC)/SX+2.*RHOM*BZ*SBKA(KA)/SX                      LJ612    361
     + +RHOM**2*SX*CKA)/CPMI                                            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(LO,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(((SIGMA(KA)/SIGAB)*(SIGMA(KB)/SIGAB))**3               LJ612    389
     + *EPSOK(KA)*EPSOK(KB))                                            LJ612    390
      TS=T/EPSAB                                                        LJ612    391
C                                                                       LJ612    392
      CALL LJBS(LANE,TS,BS,TBSP,TTBSPP,MISTAK)                          LJ612    393
C  INTERPOLATE IN THE BSTAR TABLES                                      LJ612    394
      IF(MISTAK.EQ.0)GOTO 325                                           LJ612    395
C                                                                       LJ612    396
  311 NN=311                                                            LJ612    397
      WRITE(LO,115) NN,MISTAK,LANE,TS                                   LJ612    398
      WRITE(LO,116)KA,KB,T                                              LJ612    399
      STOP                                                              LJ612    400
```

```
C  STOP IF TS IS OUTSIDE THE RANGE OF THE BSTAR TABLES
C
  325 SBKA(KA)=SBKA(KA)+SIGAB3*BS*X(KB)
C
  335 CONTINUE
C
  345 CONTINUE
C
      RHOM=RHO/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 4
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=RHO/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/EPSAB
C
      CALL LJBS(LANE,TS,BS,TBSP,TTBSPW,MISTAK)
C  INTERPOLATE IN THE BSTAR TABLES
      IF(MISTAK.EQ.0)GOTO 425
C
  421 NN=421
      WRITE(LO,115)NN,MISTAK,LANE,TS
      WRITE(LO,116)KA,KB,T
```

```
      STOP                                                              LJ612    458
C  STOP IF TS IS OUTSIDE THE INTERPOLATION TABLE                        LJ612    459
C                                                                       LJ612    460
  425 D(KA,KB)=((SC+SX*(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
C  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, RHO IN G/CM**3 AND                      LJ612    486
C  MASS WM IN GRAMS.  THE VALUE OF CZ IS ACCORDING TO                   LJ612    487
C  HIRSCHFELDER, 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)KGEOS=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 TIGEPA-440 AND IT CHANGES THE                    LJ612    514
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C  DEFAULT FACTOR 0.81**6=0.2824 IN THE CONSTANT C2.                    LJ612    515
C  THE CODE OF VAL(2) IS "SFACT" WHICH MUST BE ON                       LJ612    516
C  THE INPUT CARD AFTER "SET,LJ612,".  NOTICE THAT THE                  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 STG-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,5HLJ612,3X,6HSIGMA=,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,5HLJ612,3X,6HSIGMA=,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
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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(1H0,30X,35HTRUNCATED VIRIAL EQUATION OF STATE ,            LJ612    583
     * 18H(SUBROUTINE LJ612),/,1H ,10X,                                 LJ612    584
     * 53HSECOND VIRIAL COEFFICIENT COMPUTED FROM LENNARD-JONES,        LJ612    585
     * 15H 6-12 POTENTIAL,/,1H 10X,                                     LJ612    586
     * 52HTHIRD VIRIAL COEFFICIENT COMPUTED USING A SIMPLIFIED,         LJ612    587
     * 37H RIGID SPHERE FORMULA WITH R = SIGMA*,1PE12.5)                LJ612    588
      GOTO 1900                                                         LJ612    589
C  LANE 14 IS CALLED FROM PRINNT-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(1H0,10X,32HSTOP BY SUBROUTINE LJ612 BECAUSE,               LJ612    598
     * 25H IT WAS CALLED WITH LANE=,I5,/,1H ,10X,                       LJ612    599
     * 28HLANE 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

```
      SUBROUTINE LJBS(LANE,TS,BS,TBSP,TTBSPP,MISTAK)                    LJBS      2
C                                                                       LJBS      3
C  THIS ROUTINE PROVIDES INTERPOLATED VALUES OF BSTAR                   LJBS      4
C  AND ITS DERIVATIVES.  IT IS CALLED BY THE                            LJBS      5
C  TRUNCATED VIRIAL SUBROUTINE LJ612, BASED ON                          LJBS      6
C  LENNARD-JONES (6-12) POTENTIAL.                                      LJBS      7
C                                                                       LJBS      8
C  LANE INDICATES WHAT SHOULD BE INTERPOLATED                           LJBS      9
C           = 1 COMPUTE BSTAR AND FIRST DERIVATIVE                      LJBS     10
C           = 2 COMPUTE BSTAR AND FIRST TWO DERIVATIVES                 LJBS     11
C           = 3 COMPUTE BSTAR                                           LJBS     12
C           = 4 COMPUTE BSTAR                                           LJBS     13
C  TS       = ARGUMENT TSTAR                                            LJBS     14
C                                                                       LJBS     15
C  THE FOLLOWING WILL BE COMPUTED BY THIS ROUTINE                       LJBS     16
C                                                                       LJBS     17
C  BS       = BSTAR                                                     LJBS     18
C  TBSP     = TSTAR*(FIRST DERIVATIVE OF BSTAR)                         LJBS     19
C  TTBSPP   = TSTAR**2*(SECOND DERIVATIVE OF BSTAR)                     LJBS     20
C  MISTAK   = ERROR INDICATOR.                                          LJBS     21
C           = 0 IF NO ERROR                                             LJBS     22
C           = -1 IF TSTAR IS LESS THAN 0.01                             LJBS     23
C           = 2 IF LANE IS OUTSIDE INTERVAL (1,4)                       LJBS     24
C                                                                       LJBS     25
C  THE INTERPOLATION IS DONE IN HIRSCHFELDER-CURTIS-BIRD                LJBS     26
C  TABLES I-8 USING TWO-POINT HERMITE FORMULAS IF  0.75.LE.TS.LE.5.0 .  LJBS     27
C  OUTSIDE THIS RANGE SERIES EXPANSIONS ARE USED.                       LJBS     28
C                                                                       LJBS     29
C  AIVARS CELMINS FECIT 13 APRIL 1983.                                  LJBS     30
C                                                                       LJBS     31
      DIMENSION TRLJTB(82),BSTLJ(82),BSTLJ1(82),BSTLJ2(82)              LJBS     32
C                                                                       LJBS     33
C  THE FOLLOWING ARE HIRSCHFELDER-CURTIS-BIRD TABLES I-8                LJBS     34
C                                                                       LJBS     35
      DATA (TRLJTB(I),I=1,82) /.30, .35, .40, .45, .50, .55, .60, .65, . LJBS     36
     170, .75, .80, .85, .90, .95, 1.00, 1.05, 1.10, 1.15, 1.20, 1.25, 1 LJBS     37
     2.30, 1.35, 1.40, 1.45, 1.50, 1.55, 1.60, 1.65, 1.70, 1.75, 1.80, 1 LJBS     38
     3.85, 1.90, 1.95, 2.00, 2.10, 2.20, 2.30, 2.40, 2.50, 2.6, 2.7, 2.8 LJBS     39
     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 LJBS     40
     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, LJBS     41
     610.0, 20.0, 30.0, 40.0, 50.0, 60.0, 70.0, 80.0, 90.0, 100.0, 200.0 LJBS     42
     7, 300.0, 400.0/                                                   LJBS     43
      DATA (BSTLJ(I),I=1,82) /-27.8805010, -18.7548950, -13.7988350, -10 LJBS     44
     1.7549750, -8.7202050, -7.2740850, -6.1979708, -5.3681918, -4.71003 LJBS     45
     270, -4.1759283, -3.7342254, -3.3631193, -3.0471143, -2.7749102, -2 LJBS     46
     3.5380814, -2.3302208, -2.1463742, -1.9825492, -1.8359492, -1.70377 LJBS     47
     484, -1.5841047, -1.4752571, -1.3758479, -1.2847160, -1.2008832, -1 LJBS     48
     5.1235183, -1.0519115, -.9854534, -.9236164, -.8659428, -.8120333, LJBS     49
     6-.7615373, -.7141473, -.6695903, -.6276254, -.5506331, -.4817100, LJBS     50
     7-.4196776, -.3635757, -.3126134, -.2661334, -.2235863, -.1845073, LJBS     51
     8-.1485022, -.1152339, -.0844124, -.0557870, -.0291400, -.0042809, LJBS     52
     9.0189568, .0407201, .0611388, .0803279, .0983901, .1154169, .1319 LJBS     53
     A02, .1466837, .1610038, .1746904, .1876177, .1998951, .2115673, .2 LJBS     54
     9226751, .2332558, .2433435, .3229044, .3760885, .4134340, .4405978 LJBS     55
     C, .4608753, .5253742, .5269255, .5185750, .5083614, .4982126, .488 LJBS     56
     D6507, .4797901, .4710150, .4640695, .4114317, .3801279, .3583512/  LJBS     57
      DATA (BSTLJ1(I),I=1,82) /76.6072560, 45.2477130, 30.2670800, 21.98 LJBS     58
```

```
194820, 16.9236900, 13.5821560, 11.2488490, 9.5455096, 8.2571145, 7 LJBS
2.2540135, 6.4541400, 5.8034061, 5.2649184, 4.8127607, 4.4282616, 4 LJBS
3.0976659, 3.8106421, 3.5592925, 3.3374893, 3.1404074, 2.9642040, 2 LJBS
4.8057826, 2.6626207, 2.5326459, 2.4141403, 2.3056683, 2.2060215, 2 LJBS
5.1141772, 2.0292621, 1.9505276, 1.8773287, 1.8091057, 1.7453722, 1 LJBS
6.6857016, 1.6297207, 1.5275444, 1.4366294, 1.3552188, 1.2819016, 1 LJBS
7.2155320, 1.1551691, 1.1000353, 1.0494802, 1.0029572, .9600031, .9 LJBS
8202229, .8832774, .8488746, .8167606, .7867145, .7585430, .7320758 LJBS
9, .7071630, .6836715, .6614830, .6404922, .6206045, .6017352, .583 LJBS
A8082, .5667545, .5505118, .5350237, .5202387, .5061101, .4925951, LJBS
B.3839722, .3082566, .2524801, .2097011, .1758670, .0286638, -.0174 LJBS
C929, -.0393115, -.0516478, -.0593621, -.0645039, -.0680819, -.0706 LJBS
D470, -.0725244, -.0775400, -.0765245, -.0747534/ LJBS
 DATA (BSTLJ2(I),I=1,82) /-356.876790, -189.465360, -116.366040, -7 LJBS
18.8779500, -57.3395200, -43.8824500, -34.9186900, -28.6405000, -24 LJBS
2.0626600, -20.6131100, -17.9419000, -15.8254600, -14.1155700, -12. LJBS
37108100, -11.5398500, -10.5513300, -9.7074400, -8.9798500, -8.3470 LJBS
4000, -7.7921700, -7.3022700, -6.8669200, -6.4777700, -6.1280500, - LJBS
55.8122500, -5.5257800, -5.2648500, -5.0262800, -4.8073800, -4.6058 LJBS
6700, -4.4198000, -4.2475000, -4.0875300, -3.9386300, -3.7997200, - LJBS
73.5481400, -3.3264700, -3.1297400, -2.9540100, -2.7961400, -2.6535 LJBS
8500, -2.5241600, -2.4062300, -2.2983100, -2.1992000, -2.1078500, - LJBS
92.0234000, -1.9451100, -1.8723100, -1.8044700, -1.7410800, -1.6817 LJBS
A400, -1.6260500, -1.5737100, -1.5244100, -1.4778900, -1.4339400, - LJBS
B1.3923400, -1.3529100, -1.3154800, -1.2799100, -1.2460600, -1.2138 LJBS
C100, -1.1830500, -1.1536700, -.9193930, -.7579300, -.6398790, -.54 LJBS
D97920, -.4787790, -.1704030, -.0720120, -.0241090, .0039270, .0221 LJBS
E470, .0348170, .0440560, .0510310, .0564410, .0772960, .0813970, . LJBS
F0820550/ LJBS
C LJBS
C LJBS
      IF(LANE.GE.1.AND.LANE.LE.4)GOTO 15 LJBS
      MISTAK=2 LJBS
      RETURN LJBS
C LJBS
   15 MISTAK=0 LJBS
      IF(TS.GE.TRLJTB(10).AND.TS.LT.THLJTB(65)) GOTO 25 LJBS
      IF(TS.GE.0.01) GOTO 36 LJBS
      MISTAK=-1 LJBS
      RETURN LJBS
C LJBS
C  NEXT FIND SLOT FOR INTERPOLATION LJBS
   25 DO 35 KA=11,65 LJBS
      IF(TS.LE.TRLJTB(KA))GOTO 45 LJBS
   35 CONTINUE LJBS
C LJBS
   36 CONTINUE LJBS
C  START COMPUTING FUNCTIONS BY SERIES EXPANSION LJBS
      A1=1.225 417 702 7 * SQRT(2.)*TS**(-0.25) LJBS
      A2=-3.625 609 908 * SQRT(2.)*0.5*TS**(-0.75) LJBS
C  A1 AND A2 ARE FIRST TWO TERMS OF SERIES FOR BSTAR LJBS
      AK=-1 LJBS
      BS=A1+A2 LJBS
      TBSP=(-A1-A2*3.)/4. LJBS
      TTBSPP=(A1*5.+A2*21.)/16. LJBS
C LJBS
   37 AK=AK+1. LJBS
```

```
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
      BS=BS+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
      TTBSPP=TTBSPP+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
      TTBSPP=(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

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PAGE

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```
INPUT **TITLE,RDX SAMPLE MAY 1983 WITH LJ612 EQUATION OF STATE
INPUT **FORMULA,RDX,14710,125.71,73.5,C,3,H,6,O,6,N,6
INPUT **COMP,RDX,100
```

RDX SAMPLE MAY 1983 WITH LJ612 EQUATION OF STATE

THE COMPOSITION IS

| NAME | PERCENT BY WEIGHT | PERCENT BY MOLE | HEAT OF FORMATION (CAL/MOLE) | STANDARD VOLUME (CC/MOLE) | STANDARD ENTROPY (CAL/K/MOLE) | MOLECULAR WEIGHT | FORMULA C | H | O | N |
|---|---|---|---|---|---|---|---|---|---|---|
| RDX | 100.00 | 100.00 | 14710.00 | 125.710 | 73.500 | 222.13 | 3 | 6 | 6 | 6 |

FOR THE COMPOSITION

THE HEAT OF FORMATION IS 66.221675 CAL/GM
THE STANDARD VOLUME IS .565940 CC/GM
THE STANDARD ENTROPY IS .330893 CAL/K/GM AND
THE STANDARD ENERGY IS 66.209969 CAL/GM.

THE ELEMENTS AND PERCENT BY MOLE

| | |
|---|---|
| C | 14.29 |
| H | 28.57 |
| O | 28.57 |
| N | 28.57 |

THERE ARE 71 GASEOUS CONSTITUENTS SELECTED WITH THEIR CONSTANTS

```
          NAME    STATEO    STATER
1.)        H                2.49976   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   50614.0   33.4030
           HK= COVOLUME    40.0
           JC22 H   0.000      EPSILON/K   0.000
           JC23 H   0.000      EPSILON/K   0.000
           LJ612   SIGMA= 3.50000E+00 ANGSTROMS,   EPSILON/K= 3.00000E+02 KELVINS      (DEFAULT VALUES)
                            3.51664    .49777   -.04476    .00109   -.05409    .39615   -.06528   -1789.0   37.8110
2.)        H2
           HK= COVOLUME    80.0
           JC22 H   0.000      EPSILON/K   0.000
           JC23 H   3.340      EPSILON/K  37.000
           LJ612   SIGMA= 2.82700E+00 ANGSTROMS,   EPSILON/K= 5.97000E+01 KELVINS
3.)        N                2.50159    .19299    .07446   -.00507    .30004   -.20197    .03514   111247.0   43.1380
           HK= COVOLUME   148.0
           JC22 H   0.000      EPSILON/K   0.000
           JC23 H   0.000      EPSILON/K   0.000
           LJ612   SIGMA= 3.50000E+00 ANGSTROMS,   EPSILON/K= 3.00000E+02 KELVINS      (DEFAULT VALUES)
4.)        N2               5.43979    .21210    .02855   -.00140   -1.89542    .65127   -.07540   -4302.0   51.4860
           HK= COVOLUME   380.0
           JC22 H   0.000      EPSILON/K   0.000
           JC23 H   4.050      EPSILON/K 120.000
           LJ612   SIGMA= 3.00000E+00 ANGSTROMS,   EPSILON/K= 7.98000E+02 KELVINS
```

```
THERE ARE 21 GASEOUS CONSTITUENTS SELECTED WITH THEIR CONSTANTS

        NAME     STATEG     STATER
 5.)    NH3                8.46376   1.82197   -.44956    .03379  -4.35634   1.47414   -.17663  -18764.0   48.3899
            BKW COVOLUME    476.0
            JCZ2 R    0.000      EPSILON/K    0.000
            JCZ3 R    3.350      EPSILON/K 138.000
            LJ612    SIGMA= 2.90000E+00 ANGSTROMS,    EPSILON/K= 5.58300E+02 KELVINS
 6.)    O                  2.25142    .04450    .00726   -.00080    .33599   -.14315    .02276   58323.0   45.0630
            BKW COVOLUME    120.0
            JCZ2 R    0.000      EPSILON/K    0.000
            JCZ3 R    0.000      EPSILON/K    0.000
            LJ612    SIGMA= 3.50000E+00 ANGSTROMS,    EPSILON/K= 3.00000E+02 KELVINS      (DEFAULT VALUES)
 7.)    O2                 2.20306   1.12042   -.18485    .01276   2.02364  -1.20737    .22334   -2085.5   59.2300
            BKW COVOLUME      0.0
            JCZ2 R    0.000      EPSILON/K    0.000
            JCZ3 R    3.730      EPSILON/K 132.000
            LJ612    SIGMA= 3.46700E+00 ANGSTROMS,    EPSILON/K= 1.06700E+02 KELVINS
 8.)    C                  1.53761    .36758   -.03929    .00140    .97360   -.39914    .05551  170650.0   44.6587
            BKW COVOLUME    180.0
            JCZ2 R    0.000      EPSILON/K    0.000
            JCZ3 R    0.000      EPSILON/K    0.000
            LJ612    SIGMA= 3.50000E+00 ANGSTROMS,    EPSILON/K= 3.00000E+02 KELVINS      (DEFAULT VALUES)
 9.)    CH                 5.47939   -.14543    .02109   -.00081  -2.28410    .90814   -.11904  138395.0   48.9350
            BKW COVOLUME    420.0
            JCZ2 R    0.000      EPSILON/K    0.000
            JCZ3 R    0.000      EPSILON/K    0.000
            LJ612    SIGMA= 3.50000E+00 ANGSTROMS,    EPSILON/K= 3.00000E+02 KELVINS      (DEFAULT VALUES)
10.)    CH2                8.97406   -.19961    .00864    .00015  -4.65189   1.61523   -.20495   85688.0   46.9250
            BKW COVOLUME    525.0
            JCZ2 R    0.000      EPSILON/K    0.000
            JCZ3 R    0.000      EPSILON/K    0.000
            LJ612    SIGMA= 3.50000E+00 ANGSTROMS,    EPSILON/K= 3.00000E+02 KELVINS      (DEFAULT VALUES)
11.)    CH3                13.41149   -.74971    .07777   -.00312  -7.46014   2.31079   -.25865   19889.0   48.4680
            BKW COVOLUME    525.0
            JCZ2 R    0.000      EPSILON/K    0.000
            JCZ3 R    0.000      EPSILON/K    0.000
            LJ612    SIGMA= 3.50000E+00 ANGSTROMS,    EPSILON/K= 3.00000E+02 KELVINS      (DEFAULT VALUES)
12.)    CH4                17.83671   -.98929    .09643   -.00372 -11.42966   3.54332   -.39228  -36617.0   41.5850
            BKW COVOLUME    528.0
            JCZ2 R    0.000      EPSILON/K    0.000
            JCZ3 R    4.290      EPSILON/K 154.000
            LJ612    SIGMA= 3.75800E+00 ANGSTROMS,    EPSILON/K= 1.48600E+02 KELVINS
```

THERE ARE 21 GASEOUS CONSTITUENTS SELECTED WITH THEIR CONSTANTS

```
        NAME    STATEG    STATER
13.)    C2H2              12.44085   -.16675    .02155   -.00023  -5.90900   2.01409   -.26643   43014.0   54.7220
            BKW COVOLUME  1035.0
            JCZ2 R   0.000      EPSILON/K   0.000
            JCZ3 R   0.000      EPSILON/K   0.000
            LJ612   SIGMA= 3.50000E+00 ANGSTROMS,    EPSILON/K= 3.00000E+02 KELVINS      (DEFAULT VALUES)
14.)    C2H6              15.67150   5.06138  -1.18046    .08460  -5.78605    .91401   -.04543  -38276.2   60.1585
            BKW COVOLUME   860.0
            JCZ2 R   0.000      EPSILON/K   0.000
            JCZ3 R   0.000      EPSILON/K   0.000
            LJ612   SIGMA= 3.50000E+00 ANGSTROMS,    EPSILON/K= 3.00000E+02 KELVINS      (DEFAULT VALUES)
15.)    C3H8              45.27890  -8.45728   1.32830   -.07394 -28.09150   8.41206   -.94400  -43259.0   60.7809
            BKW COVOLUME  1280.0
            JCZ2 R   0.000      EPSILON/K   0.000
            JCZ3 R   0.000      EPSILON/K   0.000
            LJ612   SIGMA= 3.50000E+00 ANGSTROMS,    EPSILON/K= 3.00000E+02 KELVINS      (DEFAULT VALUES)
16.)    C3H8              27.28810   3.34296   -.95519    .07631 -10.21140   1.56227   -.07685  -56266.2   75.7174
            BKW COVOLUME  1280.0
            JCZ2 R   0.000      EPSILON/K   0.000
            JCZ3 R   0.000      EPSILON/K   0.000
            LJ612   SIGMA= 3.50000E+00 ANGSTROMS,    EPSILON/K= 3.00000E+02 KELVINS      (DEFAULT VALUES)
17.)    CO                 5.32449   -.18166    .02476   -.00123  -1.62632    .50286   -.05213  -30697.0   53.6070
            BKW COVOLUME   390.0
            JCZ2 R   0.000      EPSILON/K   0.000
            JCZ3 R   4.050      EPSILON/K 170.000
            LJ612   SIGMA= 3.69000E+00 ANGSTROMS,    EPSILON/K= 9.17000E+01 KELVINS
18.)    CO2               8.24460   -.09566    .01534   -.00052  -1.88500    .26808   -.01268 -101805.0   61.0700
            BKW COVOLUME   600.0
            JCZ2 R   0.000      EPSILON/K   0.000
            JCZ3 R   4.200      EPSILON/K 200.000
            LJ612   SIGMA= 3.94100E+00 ANGSTROMS,    EPSILON/K= 1.95200E+02 KELVINS
19.)    H2O               7.50251    .23407   -.03875    .00169  -4.19224   1.70652   -.23029  -63543.0   48.3880
            BKW COVOLUME   250.0
            JCZ2 R   0.000      EPSILON/K   0.000
            JCZ3 R   3.350      EPSILON/K 138.000
            LJ612   SIGMA= 2.79000E+00 ANGSTROMS,    EPSILON/K= 5.42500E+02 KELVINS
20.)    NO                 5.10888    .12763    .01842   -.00095  -1.15044    .25763   -.01367   17330.0   57.4260
            BKW COVOLUME   386.0
            JCZ2 R   0.000      EPSILON/K   0.000
            JCZ3 R   3.970      EPSILON/K 105.000
            LJ612   SIGMA= 3.49200E+00 ANGSTROMS,    EPSILON/K= 1.16700E+02 KELVINS
```

```
THERE ARE 21 GASEOUS CONSTITUENTS SELECTED WITH THEIR CONSTANTS

        NAME     STATEG     STATER
21.)     CH                4.59381    .15825   -.02096    .00079  -1.72199    .81051   -.11668    6531.0   49.5120
            BKW COVOLUME    413.0
            JCZ2 R    0.000      EPSILON/K    0.000
            JCZ3 R    0.000      EPSILON/K    0.000
            LJ612    SIGMA= 3.50000E+00 ANGSTROMS,    EPSILON/K= 3.00000E+02 KELVINS      (DEFAULT VALUES)

THERE ARE  1 CONDENSED CONSTITUENTS SELECTED WITH THEIR CONSTANTS

        NAME
 1.)     *C
            SOLID STR    .4187E+01 -.4503E+00  .8518E-01 -.4699E-02 -.1312E+01  .7536E-01  .1378E-01 -.4941E+04  .4129E+01
            STC    OLD    .4993E+01  .3963E-04  .1191E-08 -.6378E-05  .1192E-09 -.3756E-14
                          .3583E-11 -.1010E-15 0.         0.         0.         0.

INPUT **GEOS,LJ612

INPUT **EXP,RHO,1.767
** ECOMPO ERROR - STUCK IN LOCAL MINIMUM
** ECOMPO ERROR - STUCK IN LOCAL MINIMUM
** ECOMPO ERROR - ETAS EXCESSIVE ITERATIONS
```

RDX SAMPLE MAY 1983 WITH LJ612 EQUATION OF STATE PAGE 5

THE CONSTANT VOLUME EXPLOSION STATE

TRUNCATED VIRIAL EQUATION OF STATE (SUBROUTINE LJ612)
SECOND VIRIAL COEFFICIENT COMPUTED FROM LENNARD-JONES 6-12 POTENTIAL
THIRD VIRIAL COEFFICIENT COMPUTED USING A SIMPLIFIED RIGID SPHERE FORMULA WITH R = SIGMA* R.10000E-01

0 = ORIGINAL H(0) = H - ( 0.000) E(0) = E - ( 0.000) S(0) = S - ( 0.000)

| | P (ATM) | V (CC/GM) | T (K) | H(0) (CAL/GM) | E(0) (CAL/GM) | S(0) (CAL/K/GM) | VOS (CC/GM) | CV (CAL/K/GM) | ALPHA | BETA | ADEXP |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 1.) | 99941.4 | .5659 | 4365. | 1430.50 | 66.21 | 1.945 | .5659 | .453 | 2.383 | 1.234 | 2.741 |

CONSTITUENT CONCENTRATIONS - MOLES PER KGM OF EXPLOSIVE

| NAME | | 1.) |
|---|---|---|
| H2 | GAS | 13.3026 |
| H2O | GAS | 11.1692 |
| CO | GAS | 8.9822 |
| CO2 | GAS | 3.4171 |
| N2 | GAS | .7272 |
| NH3 | GAS | .3958 |
| CH4 | GAS | .0474 |
| C2H2 | GAS | .2478 |
| C2H6 | GAS | .0586 |
| C3H6 | GAS | .1142 |
| CH3 | GAS | .0484 |
| C3H4 | GAS | .0183 |
| OH | GAS | .0146 |
| H | GAS | .0020 |
| NO | GAS | .0105 |
| CH2 | GAS | .0002 |
| O2 | GAS | .0004 |
| O | GAS | .0001 |
| N | GAS | .0000 |
| CH | GAS | .0000 |
| C | GAS | .0000 |
| *C | SOLID | 0.0000 |
| TOTAL | GAS | 38.5570 |

```
INPUT **C-J+P,1+RHO+1.767
```

RDX SAMPLE MAY 1983 WITH LJ612 EQUATION OF STATE PAGE 7

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 LJ612)
SECOND VIRIAL COEFFICIENT COMPUTED FROM LENNARD-JONES 6-12 POTENTIAL
THIRD VIRIAL COEFFICIENT COMPUTED USING A SIMPLIFIED RIGID SPHERE FORMULA WITH R = SIGMA* 8.10000E-01

H = ORIGINAL H(0) = H - ( 0.000) E(0) = E - ( 0.000) S(0) = S - ( 0.000)

| | P (ATM) | V (CC/GM) | T (K) | H(0) (CAL/GM) | E(0) (CAL/GM) | S(0) (CAL/K/GM) | VGS (CC/GM) | CV (CAL/K/GM) | ALPHA | BETA | ADEXP |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 1.) | 213340.7 | .4216 | 5331. | 2617.43 | 438.99 | 1.916 | .4216 | .485 | 2.055 | 1.046 | 2.922 |

CONSTITUENT CONCENTRATIONS - MOLES PER KGM OF EXPLOSIVE

| NAME | | 1.) |
|---|---|---|
| HCN | GAS | 13.3469 |
| H2O | GAS | 10.4492 |
| CO | GAS | 5.3084 |
| CO2 | GAS | 5.5881 |
| H2 | GAS | .1333 |
| NH3 | GAS | .2701 |
| CH4 | GAS | .0080 |
| C2H2 | GAS | .3148 |
| C2H6 | GAS | .0832 |
| C3H6 | GAS | .4823 |
| CH3 | GAS | .0244 |
| C3H8 | GAS | .1113 |
| OH | GAS | .0175 |
| H | GAS | .0003 |
| NO | GAS | .0477 |
| CH2 | GAS | .0003 |
| O2 | GAS | .0062 |
| O | GAS | .0003 |
| N | GAS | .0000 |
| CH | GAS | .0001 |
| C | GAS | .0000 |
| *C | SOLID | 0.0000 |
| TOTAL | GAS | 36.1924 |

```
INPUT **STOP
09,39,41,UCLP, FATM1602C,      0.964KLNS,
```

# APPENDIX D

# INTERPOLATION FORMULAS

## APPENDIX D

## INTERPOLATION FORMULAS

In Section 6 we defined a function $\overset{*}{B}(\overset{*}{T})$ 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 $\overset{*}{B}$, $\overset{*}{B}_1$, $= \overset{*}{T} \cdot (d\overset{*}{B}/d\overset{*}{T})$ and $\overset{*}{B}_2 = \overset{*}{T}^2 \cdot (d^2\overset{*}{B}/d\overset{*}{T})$. 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

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

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:

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

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

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

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

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

and derivatives are transformed by using the chain rule

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

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

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

In order to compute $\overset{*}{B}_1 = \overset{*}{T}\,\overset{*}{B}'$ one can either interpolate $\overset{*}{B}'$ making use of the relation $\overset{*}{B}'' = \overset{*}{B}_2/\overset{*2}{T}$ or interpolate the function $\overset{*}{B}_1$ itself, or compute the derivative of Eq. (D.6), thereby disregarding the $\overset{*}{B}_2$ 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 $\overset{*}{B}_1$ is given the terms of $\overset{*}{B}_1$ and $\overset{*}{B}_2$ by the formula

$$\frac{d}{d\overset{*}{T}} \overset{*}{B}_1 = \frac{d}{d\overset{*}{T}} (\overset{*}{T}\,\overset{*}{B}') = \frac{1}{\overset{*}{T}} (\overset{*}{T}\,\overset{*}{B}' + \overset{*2}{T}\,\overset{*}{B}'') = \frac{1}{\overset{*}{T}} (\overset{*}{B}_1 + \overset{*}{B}_2) \quad . \tag{D.7}$$

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

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

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

$$\overset{*}{B}_2 = \overset{*}{T}\,\overset{*}{B}_1' - \overset{*}{B}_1 = \frac{\overset{*}{T}}{\overset{*}{T}_b - \overset{*}{T}_a} \frac{d\overset{*}{B}_1}{dx} - \overset{*}{B}_1 \quad . \tag{D.9}$$

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

$$\overset{*}{B}_2 = \overset{*}{T}\left[\frac{\overset{*}{B}_{1b} - \overset{*}{B}_{1a}}{\overset{*}{T}_b - \overset{*}{T}_a} F_1' + \frac{\overset{*}{B}_{1a} + \overset{*}{B}_{2a}}{\overset{*}{T}_a} D_0' + \frac{\overset{*}{B}_{2b} + \overset{*}{B}_{2b}}{\overset{*}{T}_b} D_1'\right] - \overset{*}{B}_1 \quad , \qquad (D.10)$$

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 $\overset{*}{B}$, four digits for $\overset{*}{B}_2$). The routine LJBS can easily be changed to produce exact function values for all $\overset{*}{T}$ by series evaluation instead of interpolation. The corresponding increase of computing time was found to be less than two percent.

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