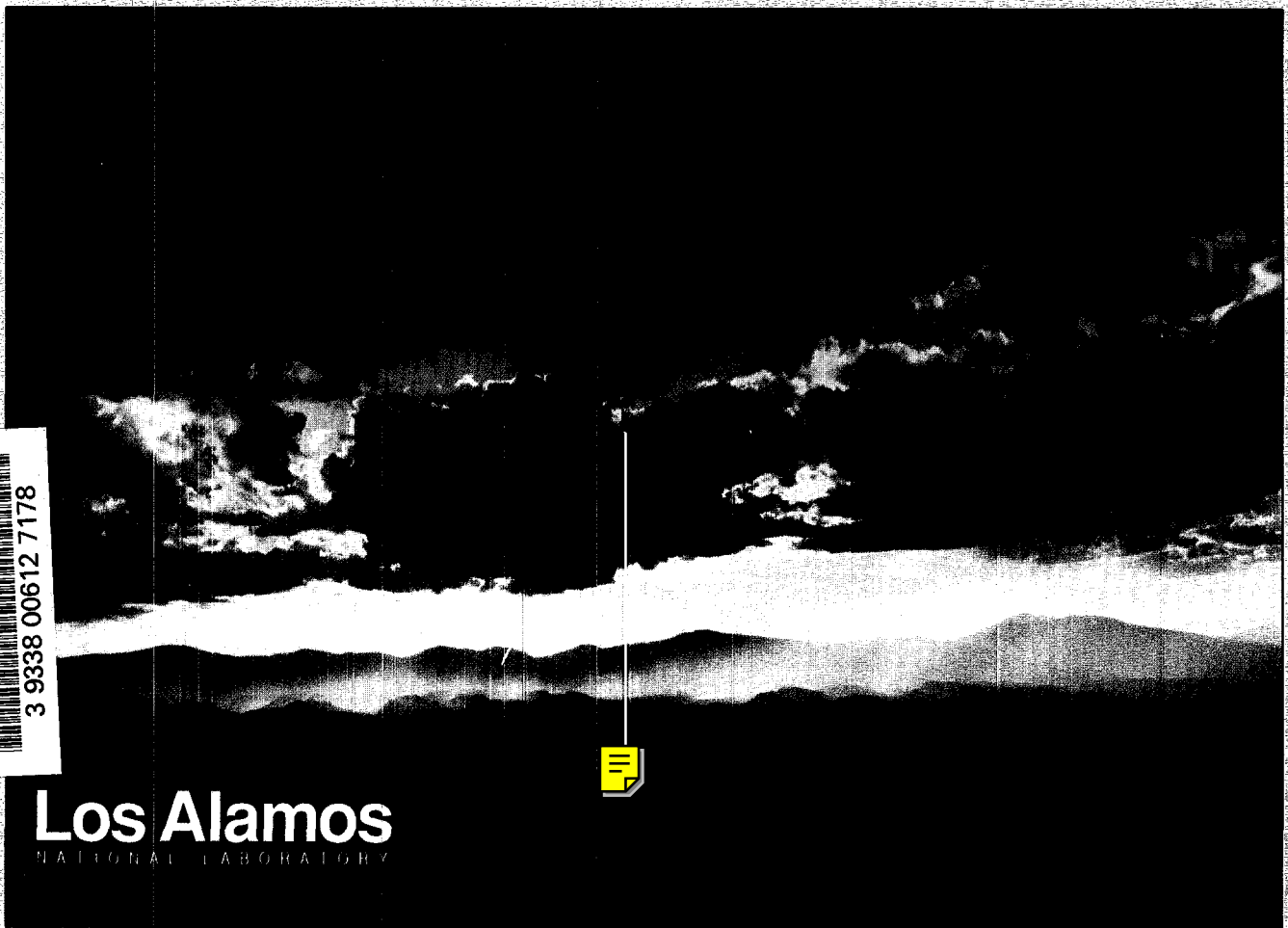


LA-UR-92-3407

**SESAME: THE LOS ALAMOS NATIONAL LABORATORY  
EQUATION OF STATE DATABASE**



LOS ALAMOS NATIONAL LABORATORY  
3 9338 00612 7178

**Los Alamos**  
NATIONAL LABORATORY

Photographer: by Chris J. Lindberg

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**SESAME: THE LOS ALAMOS NATIONAL LABORATORY  
EQUATION OF STATE DATABASE**

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**SECTION 1**  
**INTRODUCTION**

## INTRODUCTION

### THE SESAME DATABASE

The SESAME Equation-of-State (EOS) Library is a standardized, computer-based library of tables for the thermodynamic properties of materials with FORTRAN subroutines for the use of the library. All are developed and maintained by the Mechanics of Materials and Equation-of-State Group (T-1) of the Theoretical Division at Los Alamos National Laboratory.

The Library currently contains data for about 150 materials, including simple elements, compounds, metals, minerals, polymers, mixtures, etc. The EOS's for existing materials in the Library are upgraded when appropriate, and EOS's for new materials are added frequently. The Library is used by many researchers, both inside and outside the Laboratory; external users include scientists at various institutions in the United States and in other countries. The Library is presently being offered to all interested users free of charge.

The thermodynamic data stored in the Library include tables of pressure  $P$  and energy  $E$  (and also in many cases, of Helmholtz free energy  $A$ ), each as a function of density  $\rho$  and temperature  $T$ . Besides total  $P$ ,  $E$ , and  $A$  tables, often separate  $P$ ,  $E$ , and  $A$  tables of thermal electronic and ion (including zero point) contributions are available. Some materials also have vaporization, melt and shear tables. The typical density and temperature ranges are from  $10^{-6}$  to  $10^4$  gm/cc and 0 to  $10^5$  ev respectively.

There also exist SESAME Libraries for opacity and conductivity data. The lower limit on the opacity data is about 1ev. The opacity library includes Rosseland and Plank mean opacities, electron conductive opacity and mean ion charge for elements with atomic number  $Z \leq 30$ . The conductivity library contains tables of mean ion charge, electrical and thermal conductivity, thermoelectric coefficient and electron conductive opacity for elements  $Z = 1$  through  $Z = 96$ .

### THEORETICAL MODELS AND METHODS

Because of the large ranges of density and temperature, and because of the very diverse kinds of phases and materials encountered in the Library, the global EOS's in the Library are formed using various combinations of different theoretical models in different regions with interpolation between, usually thermodynamically consistent.

Most often these models include a Thomas-Fermi-Dirac theory for thermal electronic contributions to the EOS. A few EOS's incorporate the INFERNO

model for an atom embedded in an electron gas at finite temperature; electron-band structure models, including augmented plane-wave, LMTO, KKR, and Gaussian orbital approaches; or a Saha model for ionization equilibrium.

Other models include Einstein, Debye, Cowan, Chart-D and generalized Chart-D models for lattice vibrations in solids; hard-sphere perturbation approaches for fluids; and rigid-rotator and harmonic-oscillator methods for molecular rotational and vibrational terms, respectively.

Other approaches include molecular-dynamics (MD) computer simulations of metals, of rigid diatomic and triatomic molecules, and of nonrigid diatomic molecules. Pseudopotentials and melting in metals have been studied by MD. The capacity also exists in the T-1 Group to study glasses and solid-solid transitions by MD.

Various somewhat empirical methods are also used: virial expansions; analytic fits of data to various intermolecular potentials, including Lennard Jones (6,12), Buckingham (exp-6), and modified Morse potentials; multi-parameter functional fits of data; Mie-Grüneisen equation of state; etc.

The aim of the SESAME Library is to have thermodynamically self-consistent EOS's that are made with the best possible physics and the best possible agreement with available experimental data-given realistic time constraints. Most EOS's in the SESAME Library have been generated by the T-1 Group, but the Library does include some EOS's originally constructed by researchers at other institutions (such as the National Bureau of Standard and Lawrence Livermore National Laboratory and adapted by the T-1 Group for the SESAME Library). The T-1 Group uses its own versions of some externally developed theoretical models to generate EOS's, but also develops its own new models and methods.

Other features of various EOS's in the SESAME Library include treatments of shock data, incorporation of various phase transitions (including Maxwell constructions or van der Waals' loops for first-order phase transitions), modeling of foams or porous materials, and calculation of dilute gas mixtures.

Of recent interest is the inclusion of better theoretical models and methods for (1) melting and (2) nonideal mixtures in the mechanisms used to generate the global EOS's. Many of these improved models and methods have been developed by various T-1 Group members and can be used now for calculations of individual thermodynamic points or of small regions in phase space. Still other models and methods are being developed in these areas, as well as in many other areas of interest in the calculation of EOS's for a variety of diverse materials.

## SESAME SOFTWARE

### SESAME Subroutine Library

The SESAME subroutine library was developed to simplify use of tabular EOS data. SESAME tables are transmitted to users on magnetic tapes in a card image format that can be read and interpreted by the user's computing system. The user is also supplied with FORTRAN subroutines that preprocess the data into a compact binary file and update this file as needed. The user is supplied with subroutines that search this file for a given material, load data into a local array, and compute thermodynamic functions by search and interpolation. Linear and rational function interpolation schemes are available for one and two dimensions.

Routines are available to compute  $P$  and  $E$  (and their first derivatives) as a function of  $\rho$  and  $T$  and also to compute  $P$  and  $T$  (and their first derivatives) as a function of  $\rho$  and  $E$ . Other EOS data that can be computed include isotherms, isochores, adiabats, Hugoniot (shock velocities and particle velocities), vapor-liquid coexistence curves, thermodynamic behavior of foams, phase transitions, and melt and shear modulus tables.

### Display Codes

The T-1 Group has a number of in-house display codes that combine various subroutines mentioned in the preceding section to provide tabular and graphical representation of the EOS data. SES2D and SES3D are two- and three-dimensional graphics codes using DISSPLA graphics which plot tabulated data. SES2D plots isotherms, isochores, Hugoniot and adiabat. (See the end of this section for sample output from SES2D.) The SHIP code displays the library data in tabular form and the DSPLX code is used to calculate Hugoniot, isentropes, and other quantities which it also displays in tabular form. Finally, SESLIST is used to generate a catalog of materials in a SESAME library along with a description of methods used to calculate each table and its density-temperature range.

## **OBTAINING THE SESAME LIBRARY**

To obtain the SESAME EOS data and subroutine library either mail or FAX your request to

SESAME Library, T-1, MS-B221  
Los Alamos National Laboratory  
Los Alamos, NM 87545

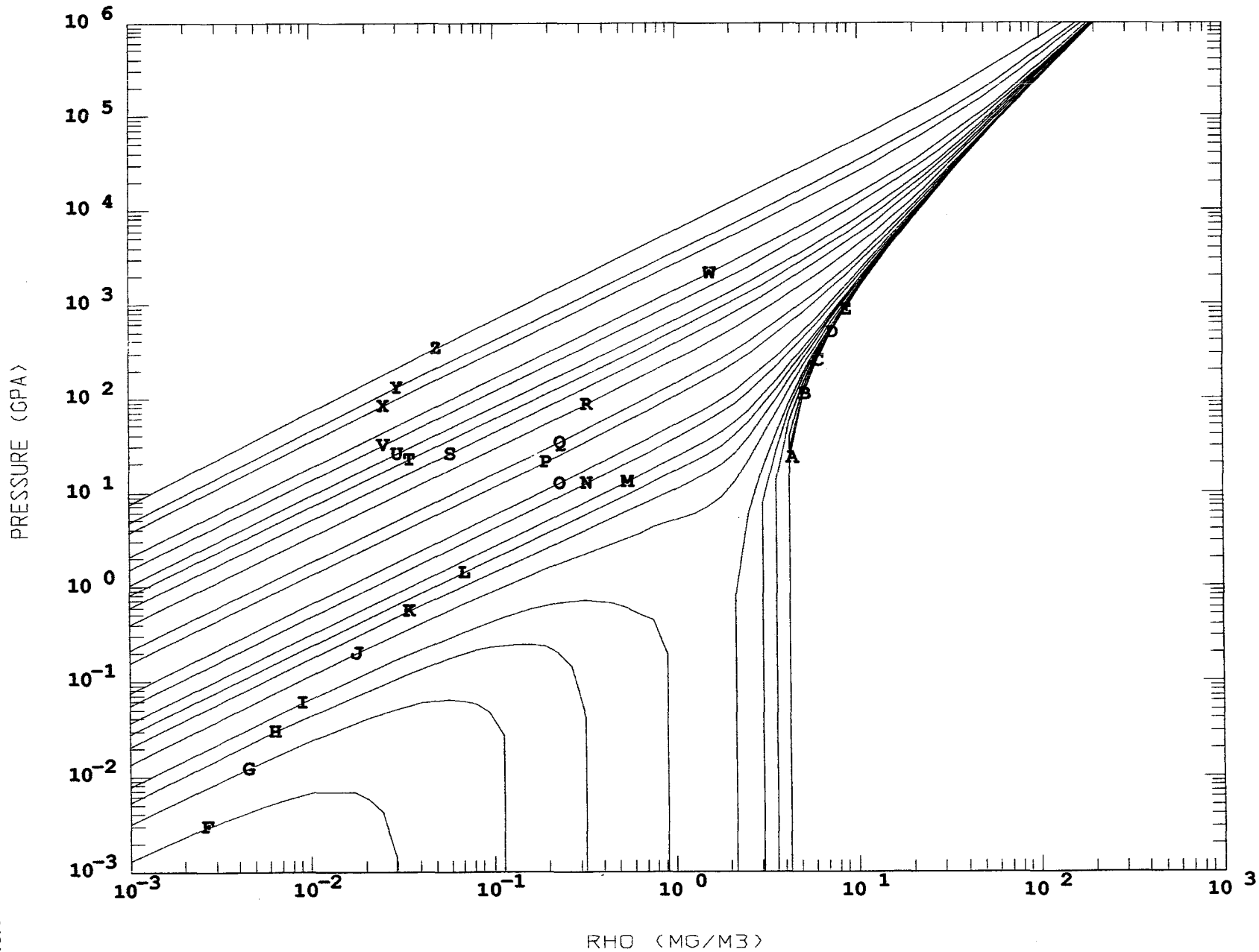
Fax No: 505-665-5757. Please include your choice of storage media and format. For a standard 2400 ft. magnetic tape specify either ASCII or EBCDIC character set and either 1600 or 6250 BPI.

Users interested in opacity data should contact

Group T-4, MS B212  
Los Alamos National Laboratory  
Los Alamos, NM 87545



7411-IST  
 TEMP (K)  
 A-0.00+00  
 B-1.45+02  
 C-2.98+02  
 D-5.80+02  
 E-1.16+03  
 F-2.90+03  
 G-5.80+03  
 H-8.70+03  
 I-1.16+04  
 J-1.74+04  
 K-2.32+04  
 L-2.90+04

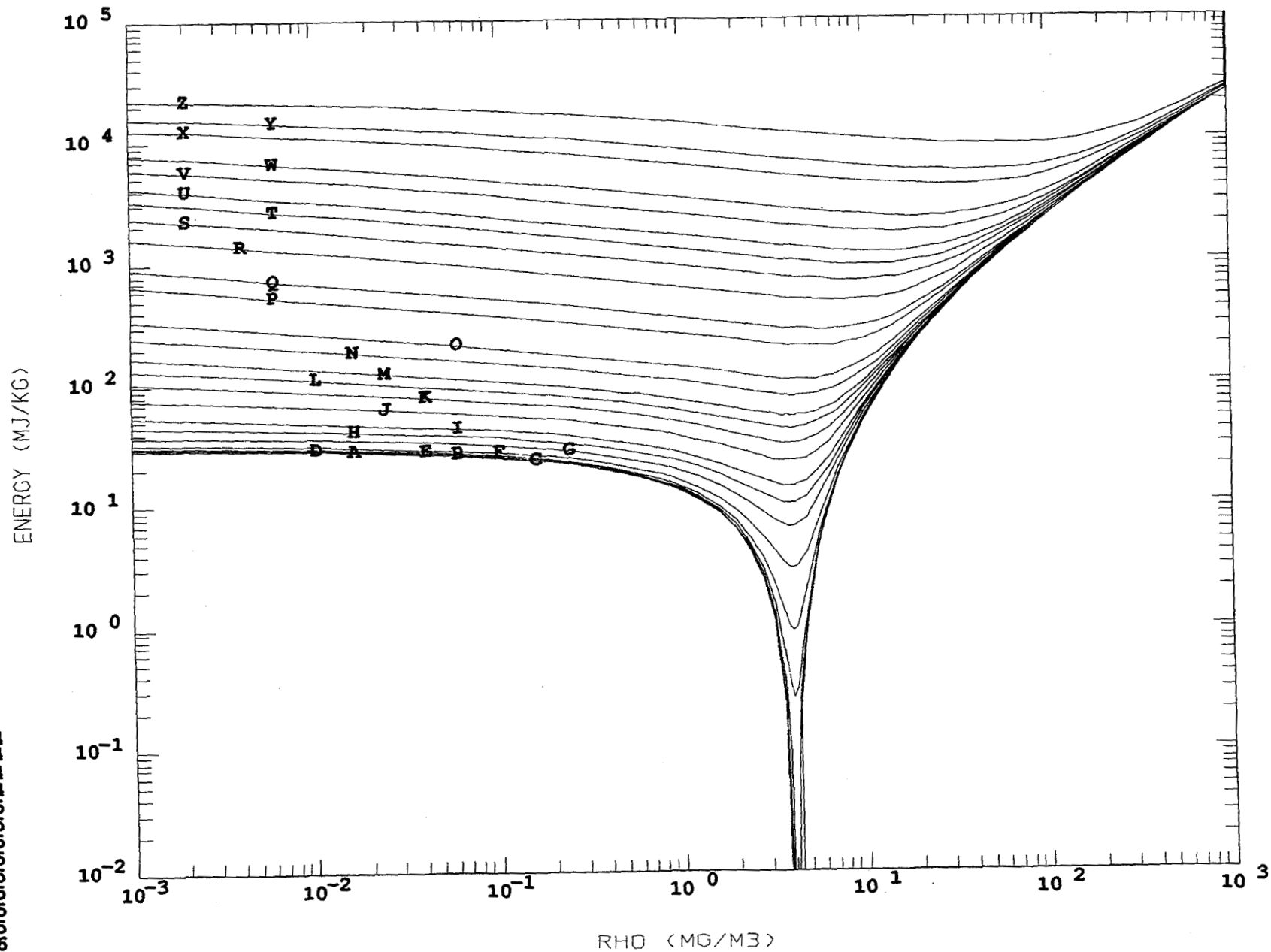


M-3.48+04  
 N-4.64+04  
 O-5.80+04  
 P-9.28+04  
 Q-1.16+05  
 R-1.74+05  
 S-2.32+05  
 T-2.90+05  
 U-3.48+05  
 V-4.64+05  
 W-5.80+05  
 X-9.28+05  
 Y-1.16+06  
 Z-1.74+06

FRIDAY 21MAY 93

TABLE 301

7411-IST  
TEMP (K)  
A-0.00+00  
B-1.45+02  
C-2.98+02  
D-5.80+02  
E-1.16+03  
F-2.90+03  
G-5.80+03  
H-8.70+03  
I-1.16+04  
J-1.74+04  
K-2.32+04  
L-2.90+04

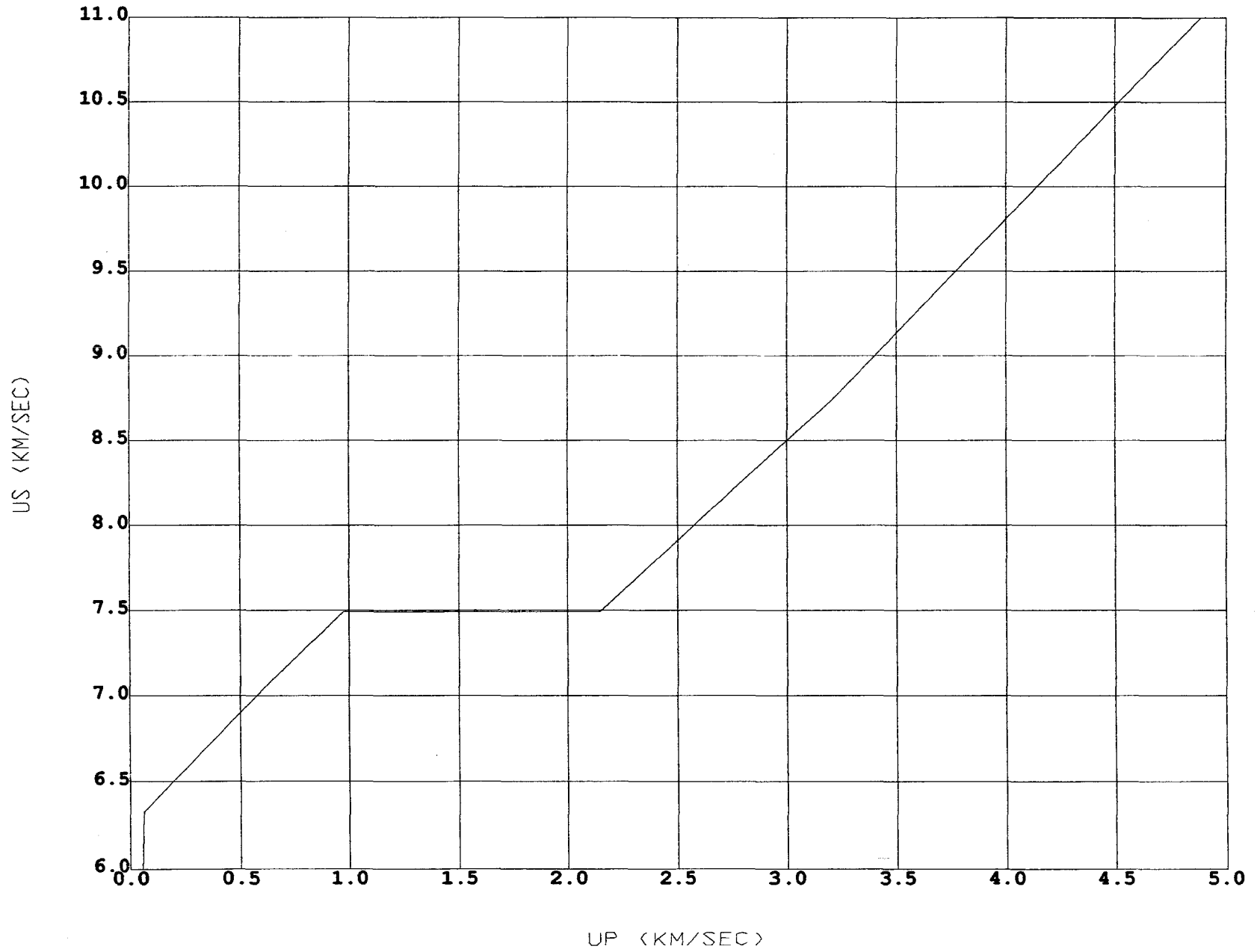


M-3.48+04  
N-4.64+04  
O-5.80+04  
P-9.28+04  
Q-1.16+05  
R-1.74+05  
S-2.32+05  
T-2.90+05  
U-3.48+05  
V-4.64+05  
W-5.80+05  
X-9.28+05  
Y-1.16+06  
Z-1.74+06

7440-HU1  
E0 MJ/KG  
0.00+00

FRIDAY 21MAY 93

TABLE 301



**SECTION 2**  
**BASELINE EOS THEORY**

## BASELINE EOS THEORY

Almost all of the equations of state being produced for SESAME are now being done with one method, one set of models. Also, over the years by far most of the EOS's have been created by similar modeling. In this section we will outline this baseline method. We will also mention a couple of more elaborate methods that are sometimes used, especially for metals. Finally, we have discontinued using a number of techniques that produced a few EOS's that are in the Library. Report LA-10160-MS should be consulted for those.<sup>(1)</sup>

The standard thinking for SESAME is that an EOS is composed of three parts; the zero temperature isotherm (cold curve), the thermal ionic, and thermal electronic. We model each separately and construct the total EOS, the 301 table, by summing the three. Other tables, 304, 305, and 306, come from the individual parts. By convention we put the zero point motion of the ions in with the thermal ionic contribution.

The thermal electronic contribution is calculated using finite temperature Thomas-Fermi-Dirac (TFD) theory. Our current model for this is due to Liberman<sup>(2)</sup> and is the same as that of Cowan and Ashkin<sup>(3)</sup> but treats exchange and correlation with a local density approximation. The thermal part is produced by running TFD everywhere including zero temperature and then subtracting the TFD cold curve from the whole table. For a few materials the INFERNO model<sup>(4)</sup> for the finite temperature electronic structure has been used. Here the Dirac equation is solved for the single particle quantum levels in the self-consistent field of an atom in a constrained spherical cell. INFERNO obtains structure from the electron ionization while TFD smoothes through such.

Our ionic models have been very similar with the current one having more details of melting.<sup>(5)</sup> The solid region is treated with Debye theory. The location of melting is determined by the Lindemann formula. Above melting an interpolation is made, going smoothly to ideal gas at high temperatures. For these models it is necessary to know the Debye temperature as a function of density. This we obtain from simple analytic forms fit to data.

For the cold curve we look at three different density regions. We usually have shock wave data from the ambient density of the solid to some high density. Over this range we use the shock data and the above fit for the Debye temperature

to calculate the cold curve from Mie-Grüneisen theory.<sup>(6)</sup> For higher densities an interpolation is made to TFD theory with a smooth connection to the Mie-Grüneisen region. For low densities a simple analytic form is again smoothly merged into the Mie-Grüneisen region. The other parameters for expansion are selected to obtain the correct cohesive energy and gas-liquid critical point. In a few special cases the Mie-Grüneisen procedure has been replaced by *ab initio* band-structure calculations.

The above method gives us our basic EOS tables. We also pull out the details of melting and vaporization and place those in special tables, 401, 411, and 412, for these phase transitions. Most recently we have included a zero temperature shear modulus table. It is sometimes appropriate to create an EOS that is a mixture. We use simple mixing rules such as additive volume and partial pressure.<sup>(7)</sup>

While the above is our standard procedure and does account, by far, for most of our database, we have and still attempt to serve the users' special needs. This includes using models and limited regions with increased accuracies as well as going to material data other than equation of state. We hope to continue this expansion of what is treated in the Sesame Library.

## REFERENCES

- (1) K. S. Holian, LANL report LA-10160-MS (1984).
- (2) D. A. Liberman, unpublished notes.
- (3) R. D. Cowan and J. Ashkin, Phys. Rev. 105, 144 (1957).
- (4) D. A. Liberman, Phys. Rev. B 20, 4981 (1979).
- (5) J. D. Johnson, High Pressure Research 6, 277 (1991).
- (6) G. I. Kerley, LANL report LA-8833-M (1981).
- (7) J. Abdallah, Jr., LANL report LA-10244-M (1984).

**SECTION 3**  
**STRUCTURE OF THE SESAME LIBRARY**



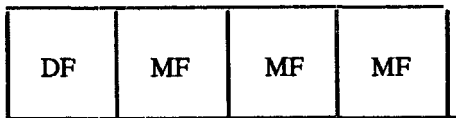
## STRUCTURE OF THE SESAME LIBRARY

The SESAME library is a fileset consisting of a directory file and one or more material files. The directory file consists of two records described on page 3-2. Each material file corresponds to a specific material and consists of an index record followed by a variable number of data records or tables. The structure of the index record appears on page 3-2. The various types of SESAME data records and their structure are shown on pages 3-3 to 3-6.

The SESAME library may be constructed with either a sequential or random I/O format. The sequential version has a one-word record mark at the end of each record, a one-word file mark at the end of each file and two end of file marks at the end of the library. The random version has an address array in the second record of the directory file with address that can be used to locate the beginning of each material file and an address array in the index record of each material file containing the addresses of the data records for that material. The random and sequential versions may be read by the TABRAN and TABSEQ subroutines found in the SESAME subroutine package described in Section 4.

The SESAME libraries maintained by T-1 on the CRAY machines at LANL have random I/O format.

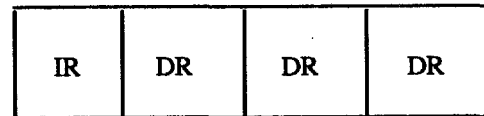
Library



DF - directory file

MF - material file

Material File



IR - index record

DR - data record

## **STRUCTURE OF THE DIRECTORY FILE FOR THE SESAME LIBRARY**

Record 1. N, DATE, VERS.

- N - Number of material files in the library (real number).
- DATE - Date of current version.
- VERS - Version number.

Record 2. (MATID(I), I = 1, N), (NWDS(I), I = 1,N), (IADR(I), I = 1, N).

- MATID - Table of material id numbers, in the same order as the material files in the library (real number).
- NWDS - For each material file MATID(I), NWDS(I) is the number of words in the index record (real number).
- IADR - IADR(I) is the address of each index record (random format).

## **STRUCTURE OF THE INDEX RECORD FOR A SESAME MATERIAL FILE**

Record 1. MATID, DATE1, DATE2, VERS, NREC, (TBLID(I), I = 1, NREC),  
(NWDS(I), I = 1 NREC), (IADR(I), I=1,NREC).

- MATID - Material id number (real number).
- DATE1 - Date of creation of material.
- DATE2 - Date when material file was last updated.
- VERS - Version number of most recent update.
- NREC - Number of data records (real number).
- TBLID - Table id numbers for the data records in the same order as they are stored in the material file.
- NWDS - For each TBLID(I), NWDS(I) is the number of words in the data record (real number).
- IADR - IADR(I) is the address of each data record (random format).

## TYPES OF SESAME DATA RECORDS

Table 101	Comments
Table 102	Comments
Table 201	Atomic Number, Atomic Mass, Normal Density
Table 301	Total EOS (304 + 305 + 306)
Table 303	Ion EOS Plus Cold Curve (305 + 306)
Table 304	Electron EOS
Table 305	Ion EOS (Including Zero Point)
Table 306	Cold Curve (No Zero Point)
Table 401	Vaporization Table
Table 411	Solid Melt Table
Table 412	Liquid Melt Table
Table 431	Shear Modulus Table
Table 501	Opacity Grid Boundary: Calculated vs. Interpolated
Table 502	Rosseland Mean Opacity ( $\text{cm}^2 \text{g}^{-1}$ )
Table 503	Electron Conductive Opacity <sup>1</sup> ( $\text{cm}^2 \text{g}^{-1}$ )
Table 504	Mean Ion Charge <sup>1</sup> (free electrons per atom)
Table 505	Planck Mean Opacity ( $\text{cm}^2 \text{g}^{-1}$ )
Table 601	Mean Ion Charge <sup>2</sup> (free electrons per atom)
Table 602	Electrical Conductivity ( $\text{sec}^{-1}$ )
Table 603	Thermal Conductivity ( $\text{cm}^{-1} \text{sec}^{-1}$ )
Table 604	Thermoelectric Coefficient ( $\text{cm}^{-1} \text{sec}^{-1}$ )
Table 605	Electron Conductive Opacity <sup>2</sup> ( $\text{cm}^2 \text{g}^{-1}$ )

<sup>1</sup>Opacity Model (Hubbard-Lampe)

<sup>2</sup>Conductivity Model (Ziman)

## STRUCTURE OF THE SESAME DATA RECORDS

**Table 201**

Word	Description	
1	ZBAR	Mean atomic number
2	ABAR	Mean atomic mass
3	RHOO	Normal (solid) density
4	B0	Solid bulk modulus
5	CEX	Exchange coefficient

**Table 301-305**

Word	Description	
1	NR	Number of densities
2	NT	Number of temperatures
3	(R(I), I=1, NR)	Density array (Mg/m <sup>3</sup> )
NR+3	(T(I), I=1, NT)	Temperature array (K)
NR+NT+3	((P(I,J), I=1, NR), J=1, NT)	Pressure array (GPa)
NR+NT+3+NR*NT	((E(I,J), I=1, NR), J=1, NT)	Energy array (MJ/kg)
NR+NT+3+2*NR*NT	((A(I,J), I=1, NR), J=1, NT)	Free energy array (MJ/kg)

**Table 306**

Word	Description	
1	NR	Number of densities
2	NT (=1)	Number of temperatures
3	(R(I), I=1, NR)	Density array (Mg/m <sup>3</sup> )
NR+3	T (=0)	Temperature (K)
NR+4	(P(I), I=1, NR)	Pressure array (GPa)
2*NR+4	(E(I), I=1, NR)	Energy array (MJ/kg)
3*NR+4	(A(I), I=1, NR)	Free energy array (MJ/kg)

**Table 401**

## Word

1	NT	Number of temperatures
2	(P(I),I=1,NT)	Vapor pressure (GPa)
2+NT	(T(I),I=1,NT)	Temperature (K)
2+2*NT	(RG(I),I=1,NT)	Vapor density on coexistence line (Mg/m <sup>3</sup> )
2+3*NT	(RL(I),I=1,NT)	Density of liquid or solid on coexistence line (Mg/m <sup>3</sup> )
2+4*NT	(EG(I),I=1,NT)	Internal energy of vapor on coexistence line (MJ/kg)
2+5*NT	(EL(I),I=1,NT)	Internal energy of liquid or solid on coexistence line (MJ/kg)
2+6*NT	(AG(I),I=1,NT)	Free energy of vapor on coexistence line (MJ/kg)
2+7*NT	(AL(I),I=1,NT)	Free energy of liquid or solid on coexistence line (MJ/kg)

**Table 411**

## Word

1	NR	Number of densities
2	NT (=1)	
3	(RS(I),I=1,NR)	Density of solid on melt line (Mg/m <sup>3</sup> )
NR+3	T (=0)	
NR+4	(TM(I),I=1,NR)	Melt temperature (K)
2*NR+4	(PM(I),I=1,NR)	Melt pressure (GPa)
3*NR+4	(ES(I),I=1,NR)	Internal energy of solid on the melt line (MJ/kg)
4*NR+4	(AS(I),I=1,NR)	Free energy of solid on the melt line (MJ/kg)

**Table 412**

## Word

1	NR	Number of densities
2	NT (=1)	
3	(RL(I),I=1,NR)	Density of liquid on melt line (Mg/m <sup>3</sup> )
NR+3	T (=0)	
NR+4	(TM(I),I=1,NR)	Melt temperature (K)
2*NR+4	(PM(I),I=1,NR)	Melt pressure (GPa)
3*NR+4	(EL(I), I=1,NR)	Internal energy of liquid on the melt line (MJ/kg)
4*NR+4	(AL(I),I=1,NR)	Free energy of liquid on the melt line (MJ/kg)

**Table 431**

Word		
2	NR	Number of densities
3	NT (=1)	
NR+3	(R(I),I=1,NR)	Density array (Mg/m <sup>3</sup> )
NR+4	T (=0)	
	(G(I),I=1,NR)	Shear modulus array (GPa)

**Table 501**

Word		
1	N	Number of temperature-density pairs
2	(T(I),R(I),I=1,N)	LOG <sub>10</sub> T <sub>1</sub> ,LOG <sub>10</sub> R <sub>1</sub> ,
		...
		LOG <sub>10</sub> T <sub>N</sub> ,LOG <sub>10</sub> R <sub>N</sub>

**Table 502-505,601-605**

Word		
1	NR	Number of densities
2	NT	Number of temperatures
3	(R(I),I=1,NR)	LOG <sub>10</sub> density array (g/cm <sup>3</sup> )
NR+3	(T(I),I=1,NT)	LOG <sub>10</sub> density array (eV)
NR+NT+3	((X(I,J),I=1,NR,)J=1,NT)	LOG <sub>10</sub> quantity

**SECTION 4**  
**USE OF THE SESAME LIBRARY**

## USE OF THE SESAME LIBRARY

In addition to the SESAME Equation of State database, the user will also receive the subroutine library SESPAC. SESPAC consists of two distinct subroutine packages. The first is composed of the basic subprograms needed to implement SESAME tables in a computer program which uses equation of state data. The second is the HYDSES subroutine package for use in hydrodynamic codes. This package is described in "HYDSES: A subroutine package for using SESAME in hydrodynamic codes" (LA-8209). In particular, we emphasize that SESPAC contains two versions of the routines ISRCHK, INV301 and RATFN1. The first version is for general EOS work. The second in each case is the HYDSES version. Note that parameters bracketed by \$ signs in dimension, common and data statements are dummy symbols to be replaced by the appropriate integer values.

There is no standard density-temperature grid for Sesame EOS tables. Each grid can be constructed to give the best representation of the EOS with as few points as possible. Consequently, storage requirements vary from material to material. At the present time, no table requires more than 15000 words. In most cases, a Sesame EOS table covers a much larger density and temperature range than is needed for a particular application. The file SESPAC provides a routine, WDW301, which reduces the size of the EOS tables by deleting data outside of specified density and temperature limits. Some users may want to call this routine from within S2GET or S2GETI. We expect that use of this option could decrease storage requirements by an order of magnitude in many cases.

The routines in the basic subroutine package are classified into several types, as shown below. These routines are written in ANS FORTRAN so that users should not have to adapt them to their local compilers. However, there may be certain exceptions to this rule. Input and output may be system dependent, so it is confined to the routines listed under A.

### A. GENERALIZED INPUT/OUTPUT.

These routines call system I/O. The user is expected to check and modify them, if necessary.

INBUF    binary read and end file test  
OUTBUF   binary write or end file mark  
INBUFR   random read  
OUTBFR   random write



OUTBUF is used to create or update the EOS Library. INBUF is used to read the library and should be compatible with OUTBUF.

## B. LIBRARY PREPROCESSOR.

Subroutine UPDATE either creates or adds data tables to a binary library file from a data tape written in ASCII/EBCDIC card image format. Although this routine is system independent, the user must provide the library file, a scratch file and a file on which the new library (created or updated) will be returned. If the user specifies the creation of a new library, the old library file is not used. If the user specifies an update to the existing library, that library remains intact after the update. It is the responsibility of the user to save the new library after execution. Usage:

CALL UPDATE (DATE, NCPW, FMT, INEW, LUP, LIB, LM, LNEW, LP)

DATE	date of updating library (a six digit real number)
NCPW	number of characters per word
FMT	format for reading Hollerith data
INEW	0 (create a new library), 1 (update an existing library)
LUP	unit number of coded update file
LIB	unit number of original library
LM	unit number of scratch file
LNEW	unit number of new (created/updated) library
LP	unit number of printer file for diagnostic messages

Externals: INBUF, OUTBUF, RDCARD, S2BLDM, RETMAT, BDINDEX, S2SRM, S2BLDL, S2UPDT, SKIPMF, COPMAT, COPMTS, S2MOD, ASORT2, UPSUM, COMPAK, UPTPGM, COMBIN, TBFCH.

Because different computing machines have different word lengths for character data, the user must supply the appropriate format for reading 80 coded characters. For example, CDC machines permit up to 10 characters per word, while IBM machines allow a maximum of 4. In these two cases, the appropriate parameters would be as follows.

CDC: NCPW = 10, FMT = "(8A10)"  
IBM: NCPW = 4, FMT = "(20A4)"

## C. PACKAGED EOS ROUTINES FOR HYDRO CODES.

**S2GET, S2EOS** - These routines are intended for hydro codes which use density and temperature as the independent variables and pressure and internal energy as the dependent variables.

**S2GET:** Subroutine S2GET is used to get data from the library. S2GET reads in the 201 and 301 tables for the material specified.

The user must allocate an array for storage of the EOS tables and provide a COMMON block for a directory to this array. The COMMON block has the form

```
COMMON/S2DIR/LCMX, NRS, LCFW (10)
```

LCMX     length of the array  
NRS      number of material regions (see below)  
LCFW     an array used as a directory, initialized to zero by the user

Usage of S2GET is as follows:

```
CALL S2GET (IR, IDS2, TBLS, LCNT, LU, IFL)
```

IR        material region number  
IDS2     Sesame material number  
TBLS     name of array designated for storage of tables  
LCNT     current word in array TBLS  
LU        unit number for library  
IFL      error flag

Each "region" corresponds to a different material. Regions should be numbered consecutively, whether or not a Sesame EOS is used. The same EOS may be requested for more than one region -- the routine will load a given table only once. S2GET must be called once for each region for which a Sesame EOS is required.

Data is loaded into the array TBLS, beginning with the word TBLS (LCNT). After successful execution of the routine, LCNT is set to the first word location following the data string which has been loaded. S2GET can be called again, using this new value of LCNT. However, the user can load other data into the array and compute a new value of LCNT before calling S2GET

again. If the routine is successful,  $IFL = 1$  is returned. If  $IFL = 0$ , S2GET was unable to locate the EOS tables on the file LU. If  $IFL < 0$ , there is insufficient storage in the array TBLs, and the size of the array should be increased by at least  $|IFL|$  words. This feature will enable some users to allocate storage dynamically.

**S2EOS:** Subroutine S2EOS is used to compute an EOS point. That is, it computes the pressure, energy, and their derivatives for a given density and temperature. Usage:

CALL S2EOS (IR, TBLs, R, T, P, E)

IR            material region number  
TBLs        name of array which contains the EOS tables  
R            density in  $\text{Mg/m}^3$   
T            temperature in degrees Kelvin  
P, E        pressure, internal energy vectors

P(1), E(1) pressure in GPa, internal energy in MJ/kg  
P(2), E(2) density derivatives,  $(\partial P/\partial \rho)_T$ ,  $(\partial E/\partial \rho)_T$   
P(3), E(3) temperature derivatives,  $(\partial P/\partial T)_\rho$ ,  $(\partial E/\partial T)_\rho$

Externals: INBUF, TBFCH, LA301A, ISRCH, RATFN2.

The parameters IR and TBLs should be identical to those which were used in calling S2GET. Note that the region number, not the Sesame material number, is used to identify the particular EOS table.

These programs are particularly useful for hydrodynamic codes. They provide for computations involving several Sesame tables, for the use of Sesame tables along with other EOS options, and for the specification of the same Sesame table in more than one region. All the necessary bookkeeping is internal to the routines.

S2GETI, S2EOSI - These routines are to be incorporated into a hydro code which uses the inverted form of an equation of state. Density and internal energy are the independent variables, and pressure and temperature are the dependent variables.

These routines are very similar to those described above. Usage of S2GETI is identical to S2GET. However, S2GETI reformats the EOS tables in order to

make the computations with S2EOSI more efficient. Usage of S2EOSI is as follows:

CALL S2EOSI (IR, TBLs, R, E, P, T)

IR material region number  
TBLs name of array which contains the EOS tables  
R density in Mg/m<sup>3</sup>  
E internal energy in MJ/kg  
P, T pressure, temperature vectors

P(1), T(1) pressure in GPa, temperature in Kelvins,  
P(2), T(2) density derivatives,  $(\partial P/\partial \rho)_E$ ,  $(\partial T/\partial \rho)_E$   
P(3), T(3) energy derivatives,  $(\partial P/\partial E)_\rho$ ,  $(\partial T/\partial E)_\rho$ .

Externals: INBUF, TBFCH, LA302A, INV301, ISRCH, ISRCHK,  
RATFN1, RATFN2.

For certain materials, the library also has tables of the pressure, temperature, density, and internal energy along the vapor-liquid coexistence curve. This information is needed in reactor safety problems. Routines S2GET and S2GETI can be modified to access the coexistence data, and routine LA401A can be used to compute the thermodynamic quantities.

#### D. AUXILIARY PACKAGED ROUTINES.

S2HUGI - Compute point on a Hugoniot  
S2SHKI - Compute point on a Hugoniot  
S2ABTI - Compute point on an Adiat

#### E. SEARCH AND INTERPOLATION.

Basic routines to operate on data strings read in from library. Not usually called directly - LA301A, LA302A, WDW301, INV301, ISRCH, ISRCHK, RATFN1, RATFN2, LA401A, LA302B, LA302S.

RATFN1 and RATFN2 are the 1- and 2-dimensional rational function interpolation routines. RATFN2 also has a bilinear interpolation option.

## F. LIBRARY MANIPULATION.

Basic routines to get data from a library. Not usually called directly - TBFCH, TABRAN, COPMAT, RDCARD, SKIPMF, COPMTS, LIBNIT.

In the basic subroutine package, OUTBUF is used to create a sequentially formatted library. Tables are then fetched from this library using TBFCH which calls INBUF. A random formatted library may be created by using OUTBFR instead of OUTBUF. Tables may be fetched from the random library using TABRAN which calls INBUFR. (The routines TABSEQ and TABFCH in the HYDSES package may also be used to read SESAME tables. See LA-8209 for their usage.)

## G. TEST PROBLEM.

To test the above procedures and to illustrate use of the Sesame library, we have constructed a test problem. - Subroutine TPRB1 accesses data for several materials specified by the user and computes and prints Hugoniot curves. Usage:

CALL TPRB1 (IDS2, N, LU, LP)

IDS2	An array, of dimension N, giving the material numbers selected by the user
N	number of materials specified
LU	unit number for library
LP	unit number for line printer

Externals: S2GETI, S2SHKI.

At the end of this section is a sample of the output from this routine, called with the following material numbers.

IDS2(1) = 3200 (lead),  
IDS2(2) = 3332 (copper),  
IDS2(3) = 3717 (aluminum).

(LCMX = 45000 in TPRB1)

The output variables are as follows.

R density in Mg/m<sup>3</sup>,  
P pressure in GPa,  
E internal energy in MJ/kg,  
T temperature in degrees Kelvin,  
US shock velocity in km/sec,  
UP particle velocity in km/sec.

## shock hugoniot for sesame material number 3200

r mg/m3	p gpa	e mj/kg	t kelvin	us km/sec	up km/sec
0.158e+02	0.400e+02	0.500e+00	0.152e+04	0.353e+01	0.100e+01
0.190e+02	0.113e+03	0.200e+01	0.770e+04	0.497e+01	0.200e+01
0.217e+02	0.214e+03	0.450e+01	0.168e+05	0.628e+01	0.300e+01
0.242e+02	0.341e+03	0.800e+01	0.278e+05	0.753e+01	0.400e+01
0.264e+02	0.497e+03	0.125e+02	0.396e+05	0.876e+01	0.500e+01
0.284e+02	0.680e+03	0.180e+02	0.533e+05	0.999e+01	0.600e+01
0.301e+02	0.891e+03	0.245e+02	0.687e+05	0.112e+02	0.700e+01
0.318e+02	0.113e+04	0.320e+02	0.824e+05	0.124e+02	0.800e+01

## shock hugoniot for sesame material number 3332

r mg/m3	p gpa	e mj/kg	t kelvin	us km/sec	up km/sec
0.109e+02	0.496e+02	0.500e+00	0.367e+03	0.555e+01	0.100e+01
0.125e+02	0.125e+03	0.200e+01	0.214e+04	0.699e+01	0.200e+01
0.137e+02	0.231e+03	0.450e+01	0.494e+04	0.863e+01	0.300e+01
0.147e+02	0.363e+03	0.800e+01	0.937e+04	0.102e+02	0.400e+01
0.157e+02	0.517e+03	0.125e+02	0.155e+05	0.116e+02	0.500e+01
0.166e+02	0.694e+03	0.180e+02	0.219e+05	0.130e+02	0.600e+01
0.175e+02	0.892e+03	0.245e+02	0.288e+05	0.143e+02	0.700e+01
0.184e+02	0.111e+04	0.320e+02	0.364e+05	0.156e+02	0.800e+01

## shock hugoniot for sesame material number 3717

r mg/m3	p gpa	e mj/kg	t kelvin	us km/sec	up km/sec
0.318e+01	0.180e+02	0.500e+00	0.494e+03	0.667e+01	0.100e+01
0.360e+01	0.432e+02	0.200e+01	0.112e+04	0.800e+01	0.200e+01
0.399e+01	0.753e+02	0.450e+01	0.247e+04	0.930e+01	0.300e+01
0.434e+01	0.114e+03	0.800e+01	0.460e+04	0.106e+02	0.400e+01
0.467e+01	0.160e+03	0.125e+02	0.736e+04	0.119e+02	0.500e+01
0.497e+01	0.213e+03	0.180e+02	0.108e+05	0.131e+02	0.600e+01
0.525e+01	0.272e+03	0.245e+02	0.149e+05	0.144e+02	0.700e+01
0.552e+01	0.338e+03	0.320e+02	0.195e+05	0.157e+02	0.800e+01
0.577e+01	0.411e+03	0.405e+02	0.246e+05	0.169e+02	0.900e+01
0.601e+01	0.490e+03	0.500e+02	0.301e+05	0.182e+02	0.100e+02
0.624e+01	0.576e+03	0.605e+02	0.358e+05	0.194e+02	0.110e+02
0.647e+01	0.668e+03	0.720e+02	0.416e+05	0.206e+02	0.120e+02
0.668e+01	0.766e+03	0.845e+02	0.478e+05	0.218e+02	0.130e+02
0.688e+01	0.871e+03	0.980e+02	0.543e+05	0.230e+02	0.140e+02
0.707e+01	0.983e+03	0.112e+03	0.611e+05	0.243e+02	0.150e+02
0.726e+01	0.110e+04	0.128e+03	0.682e+05	0.255e+02	0.160e+02

## PUBLICATIONS, 1979-1992

### Journal Articles

- R. C. Albers, M. A. Boring, and J. C. Boettger, "LDA Applications to the Properties of Periodic Systems," *Adv. in Quant. Chem.* **21**, 365 (1990).
- R. C. Albers, M. Alouani, J. M. Wills, and M. Springborg, "Electronic Properties of Mixed-Valence Pt-BR Chains," *Synthetic Metals* **41-43**, 2739 (1991).
- G. A. Baker, Jr., and J. D. Johnson, "General Structure of the Thomas-Fermi Equation of State," *Phys. Rev. A* **44**, 2271 (1991).
- B. I. Bennett and D. A. Liberman, "Quantum Mechanical Effects on the Shock Hugoniot," *Shock Compression of Condensed Matter - 1991*, S. C. Schmidt, R. D. Dick, J. W. Forbes, D. G. Tasker (eds.) (Elsevier Science Publishing Company, New York, 1992) p. 49.
- J. C. Boettger and S. B. Trickey, "Total Energy and Pressure in the Gaussian-Orbitals Technique. I. Methodology with Application to the High-Pressure Equation of State of Neon," *Phys. Rev. B* **29**, 6425 (1984).
- J. C. Boettger and S. B. Trickey, "Total Energy and Pressure in the Gaussian-Orbitals Technique. II. Pressure-Induced Crystallographic Phase Transition and Equilibrium Properties of Aluminum," *Phys. Rev. B* **29**, 6434 (1984).
- J. C. Boettger and S. B. Trickey, "Equation of State of Properties of Lithium," *Phys. Rev. B* **32**, 3391 (1985).
- J. C. Boettger, "Equation of State and Metalization of Neon," *Phys. Rev. B* **33**, 6788 (1986).
- J. C. Boettger and R. C. Albers, "Structural Phase Stability in Lithium to Ultrahigh Pressures," *Phys. Rev. B* **39**, 3010 (1989).
- J. C. Boettger, S. B. Trickey, and J. A. Nobel, "Comment on 'Total Energy Calculations of Solid H, Li, Na K, Rb, and Cs,'" *Phys. Rev. B* **45**, 7503 (1992).
- R. D. Dick and G. I. Kerley, "Shock Compression Data for Liquids. II. Condensed Hydrogen and Deuterium," *J. Chem. Phys.* **73**, 5264 (1980).
- Olle Eriksson and J. M. Wills, "Theoretical Aspects of the  $5f$  Delocalization of Americium Under Pressure," *Phys. Rev. B* **45**, 3198 (1992-I).
- Olle Eriksson, J. M. Wills, and Per Söderlind, " $fcc \rightarrow bct$  Phase Transition in Th at Extreme Compressions: Theory," *Phys. Rev. B* **45**, 12588 (1992).
- N. R. Greiner, D. S. Phillips, J. D. Johnson, and F. Volk, "Diamonds in Detonation Soot," *Nature* **333**, 440 (1988).
- W. A. Harrison and J. M. Wills, "Interionic Interactions in Simple Metals," *Phys. Rev. B* **25**, 5007 (1982).
- W. A. Harrison and G. K. Straub, "Electronic Structure and Properties in d- and f-shell Metal Compounds," *Phys. Rev. B* **36**, 2695 (1987).
- B. L. Holian and G. K. Straub, "Molecular Dynamics of Shock Waves in One-Dimensional Chains," *Phys. Rev. B* **18**, 1593 (1978).
- B. L. Holian and G. K. Straub, "Molecular Dynamics of Shock Waves in Three-Dimensional Solids: Transition from Non-steady to Steady Waves in Perfect Crystals and Implications for the Rankine-Hugoniot Conditions," *Phys. Rev. Lett.* **43**, 1598 (1979).
- B. L. Holian, W. G. Hoover, B. Moran and G. K. Straub, "Shockwave Structure via Nonequilibrium Molecular Dynamics and Navier-Stokes Continuum Mechanics," *Phys. Rev. A* **22**, 2498 (1980).



- B. L. Holian, G. K. Straub, R. E. Swanson, and D. C. Wallace, "Melting of Pseudopotential Sodium from Molecular Dynamics," *Phys. Rev. B* **27**, 2873 (1983).
- J. D. Johnson and J. C. Bonner, "Excitation Spectrum and Thermodynamic Properties of the Ising-Heisenberg Linear Ferromagnet," *Phys. Rev. Lett.* **44**, 616 (1980).
- J. D. Johnson and J. C. Bonner, "Excitation Spectrum and Low-Temperature Thermo-dynamics of the Ising-Heisenberg Linear Ferro-magnet," *Phys. Rev. B* **22**, 251 (1980).
- J. D. Johnson, "A Survey of Analytic Results for the 1-D Heisenberg Magnets," *J. Appl. Phys.* **52**, 1991 (1981).
- J. D. Johnson, "A Comment on the Equation of State by Hirschfelder et al.," *AIChE Journal* **27**, 166 (1981).
- J. D. Johnson, M. S. Shaw, and B. L. Holian, "Dense Molecular Thermodynamics," *Shock Waves in Condensed Matter - 1983*, J. R. Asay, R. A. Graham, G. K. Straub (eds.) (Elsevier Science Publishing Company, New York, 1984) p.27.
- J. D. Johnson, M. S. Shaw, and B. L. Holian, "The Thermodynamics of Dense Fluid Nitrogen by Molecular Dynamics," *J. Chem. Phys.* **80**, 1279 (1984).
- J. D. Johnson and M. S. Shaw, "Thermodynamics Using Effective Spherical Potentials for CO<sub>2</sub> Anisotropies," *J. Chem. Phys.* **83**, 1271 (1985).
- J. D. Johnson, "Carbon in Detonations," *Proceedings of Ninth Symposium (International) on Detonation*, W. J. Morat (ed.) (OCNR 113291-7, Arlington, Virginia, 1989) p. 417.
- J. D. Johnson, "A Generic Model for the Ionic Contribution to the Equation of State," *High Pressure Research* **6**, 277 (1991).
- J. N. Johnson, "Calculated Shock Pressures in the Aquarium Test," *Shock Waves in Condensed Matter - 1981*, W. J. Nellis, L. Seaman, R. A. Graham (eds.) (Am. Inst. of Phys., New York, 1982) p. 568.
- J. N. Johnson and Selma Goldstein, "Aquarium Tests on Aluminized ANFO," *Seventh Symposium (International) on Detonation*, J. M. Short (ed.) (NSWC MP82-334, Silver Spring, Maryland, 1982) p. 1016.
- J. N. Johnson, C. L. Mader, and S. Goldstein, "Performance Properties of Commercial Explosives," *Propellants, Explosives, and Pyrotechnics* **8**, 8 (1983).
- J. N. Johnson, P. S. Lomdahl, and J. M. Wills, "Analysis of Internal Stress and Anelasticity in the Shock-Compressed State From Unloading Wave Data," *Acta Metall.* **39**, 3015 (1991).
- J. N. Johnson and P. S. Lomdahl, "Anelastic Release From the Shock-Compressed State," *J. de Physique IV, Colloque C3*, 223 (1991).
- J. N. Johnson, R. S. Hixson, G. T. Gray III, and C. E. Morris, "Quasi-Elastic Release in Shock-Compressed Solids," *J. Appl. Phys.* **72**, 429 (1992).
- G. I. Kerley, "Perturbation Theory and the Thermodynamic Properties of Fluids. I. General Theory," *J. Chem. Phys.* **73**, 469 (1980).
- G. I. Kerley, "Perturbation Theory and the Thermodynamic Properties of Fluids. II. The CRIS Model," *J. Chem. Phys.* **73**, 478 (1980).
- G. I. Kerley, "Perturbation Theory and the Thermodynamic Properties of Fluids. III. In-verse Power and 6-12 Potentials," *J. Chem. Phys.* **73**, 487 (1980).
- G. I. Kerley, "A Theoretical Equation of State for Methane," *J. Appl. Phys.* **51**, 5368 (1980).

- G. I. Kerley and J. Abdallah, Jr., "Theoretical Equations of State for Molecular Fluids: Nitrogen, Oxygen, and Carbon Monoxide," *J. Chem. Phys.* **73**, 5337 (1980).
- D. S. King, B. E. Freeman, D. D. Eilers, and J. D. Johnson, "The Effective Yield of a Nuclear Explosion in a Small Cavity in Geo-logic Material: Enhanced Coupling Revisited," *J. Geophys. Res.* **94**, 12375 (1989).
- D. A. Liberman, "Self-Consistent Field Model for Condensed Matter," *Phys. Rev. B* **20**, 4981 (1979).
- D. A. Liberman, "INFERNO: A Better Model of Atoms in Dense Plasmas," *J. Quant. Spectrosc. Radiat. Transfer* **27**, 335 (1982).
- D. A. Liberman and B. I. Bennett, "Atomic Vibrations in a Self-Consistent Field Atom-in-Jellium Model of Condensed Matter," *Phys. Rev. B* **42**, 2475 (1990).
- D. MacGowan, J. D. Johnson, and M. S. Shaw, "Angular Correlations in Dense Hot Diatomic Fluids," *J. Chem. Phys.* **82**, 3765 (1985).
- D. S. Moore, S. C. Schmidt, M. S. Shaw, and J. D. Johnson, "CARS Spectroscopy of Shock-Compressed Liquid Nitrogen," *J. Chem. Phys.* **90**, 1368 (1989).
- G. A. Rinker and B. I. Bennett, "Electrical Resistivities of Dense Plasmas," *IEEE International Conference on Plasma Science (Publishing Services IEEE, New York, 1981)* p.95.
- S. C. Schmidt, D. S. Moore, M. S. Shaw, and J. D. Johnson, "Vibrational Spectroscopy of Shock-Compressed Fluid N<sub>2</sub> and O<sub>2</sub>," *Shock Waves in Condensed Matter - 1987*, S. C. Schmidt, N. C. Holmes (eds.) (Elsevier Science Publishing Company, New York, 1988) p. 489, and *Proceedings of XI AIRAPT International High-Pressure Conference, Kiev, USSR, July 12-17 (1987)*.
- S. C. Schmidt, D. S. Moore, M. S. Shaw, and J. D. Johnson, "Coherent Anti-Stokes Raman Spectroscopy of Shock-Compressed Liquid Oxygen," *J. Chem. Phys.* **91**, 6765 (1989).
- G. L. Schott, M. S. Shaw, and J. D. Johnson, "Shocked States from Initially Liquid Oxygen-Nitrogen Systems," *J. Chem. Phys.* **82**, 4264 (1985).
- M. S. Shaw, J. D. Johnson, and B. L. Holian, "Effective Spherical Potentials for Molecular Fluid Thermodynamics," *Phys. Rev. Lett.* **50**, 1141 (1983).
- M. S. Shaw and J. D. Johnson, "A Temperature Independent Spherical Potential Which Reproduces Exactly the Second Virial Coefficient of Non-Polar Molecules," *J. Chem. Phys.* **81**, 3360 (1984).
- M. S. Shaw and J. D. Johnson, "The Theory of Dense Molecular Fluid Equations of State with Application to Detonation Products," *Proceedings 8th Symposium (International) on Detonation*, J. M. Short (ed.) (NSWC MP86-194, Silver Spring, Maryland, 1985) p. 531.
- M. S. Shaw, J. D. Johnson, and J. D. Ramshaw, "An Approximate Variational Method for Improved Thermodynamics of Molecular Fluids," *J. Chem. Phys.* **84**, 3479 (1986).
- M. S. Shaw and J. D. Johnson, "Carbon Clustering in Detonations," *J. Appl. Phys.* **62**, 2080 (1987).
- M. S. Shaw and J. D. Johnson, "Carbon Clustering in Detonations," *Proceedings of the International Symposium on Pyrotechnics and Explosives*, Ding Jing (ed.), (Beijing, China, 1987) p. 644.
- G. K. Straub, B. L. Holian, and R. G. Petschek, "Molecular Dynamics of Shock Waves in One-Dimensional Chains. II. Thermalization," *Phys. Rev. B* **19**, 4049 (1979).

- G. K. Straub, R. E. Swanson, B. L. Holian, and D. C. Wallace. "The Thermal Properties of Metallic Sodium Near Melt from Molecular Dynamics Calculations," *Proceedings of the CECAM Workshop on "Ab Initio Calculations of Phonon Spectra,"* J. T. Devreese, V. Van Doren, P. Van Camp (eds.) (Plenum Press, New York, 1982) p. 137.
- G. K. Straub, S. Schiferl, and D. C. Wallace, "Thermodynamic Properties of Fluid Sodium from Molecular Dynamics Calculations," *Phys. Rev. B* **28**, 312 (1983).
- G. K. Straub and D. C. Wallace, "Thermodynamic Calculations for bcc Sodium at High Pressures," *Phys. Rev. B* **30**, 3929 (1984).
- G. K. Straub and W. A. Harrison, "Analytic Methods for the Calculation of Electronic Structure of Solids," *Phys. Rev. B* **31**, 6155 (1985).
- G. K. Straub, "The Overlap of Electron Core States for Very High Compressions," *Shock Waves in Condensed Matter - 1985*, Y. M. Gupta (ed.) (Plenum Press, New York, 1985) p. 85.
- G. K. Straub, "Thermodynamics of Metallic Solids and Fluids from Molecular Dynamics," *Computer Simulation in Materials Science*, R. J. Arsenault, J. R. Beeler (eds.) (American Society for Metals, Metals Park, Ohio, 1986) p. 79.
- G. K. Straub, J. M. Wills, and D. C. Wallace, "Elastic Moduli of Copper Under Compression," *Shock Waves in Condensed Matter - 1987*, S. C. Schmidt, N. C. Holmes (eds.) (Elsevier Science Publishing Company, New York, 1988) p. 207.
- G. K. Straub and W. A. Harrison, "Self-Consistent Theory of Elasticity in Ionic Solids," *Phys. Rev. B* **39**, 10325 (1989).
- G. K. Straub, "Extrapolation of the Shear Modulus to High Compressions and Negative Pressures," *Shock Waves in Condensed Matter - 1991*, S. C. Schmidt, R. Dick (eds.) (Elsevier Science Publishing Company, New York, 1992) p. 391.
- R. E. Swanson, G. K. Straub, B. L. Holian, and D. C. Wallace, "Thermodynamic Properties of Solid Sodium from Quasiharmonic Lattice Dynamics and Molecular Dynamics," *Phys. Rev. B* **25**, 7807 (1982).
- R. E. Swanson, G. K. Straub, and B. L. Holian, "Molecular Dynamics of Sodium Using a Model Pseudopotential," *Shock Waves in Condensed Matter - 1981*, W. J. Nellis, L. Seaman, R. A. Graham (eds.) (American Institute of Physics, New York, 1982).
- D. C. Wallace, B. L. Holian, J. D. Johnson, and G. K. Straub, "A High-Temperature Free-Energy Expansion for Metal Fluids," *Phys. Rev. A* **26**, 2882 (1982).
- D. C. Wallace and G. K. Straub, "Ensemble Corrections for the Molecular Dynamics Ensemble," *Phys. Rev. A* **27**, 2201 (1983).
- D. C. Wallace, S. Schiferl, and G. K. Straub, "Stresses and Elastic Constants of Metals with Classical Ion Motion," *Phys. Rev. A* **30**, 616 (1984).
- J. M. Wills and W. A. Harrison, "Interionic Interactions in Transition Metals," *Phys. Rev. B* **28**, 4363 (1983).
- J. M. Wills and W. A. Harrison, "Further Studies on Interionic Interactions in Simple Metals and Transition Metals," *Phys. Rev. B* **29**, 5486 (1984).
- J. M. Wills and B. R. Cooper, "Synthesis of Band and Model Hamiltonian Theory for Hybridizing Cerium Systems," *Phys. Rev. B* **36**, 3809 (1987).
- J. M. Wills and B. R. Cooper, "First Principles Calculations for a Model Hamiltonian Treatment of Hybridizing Light Actinide Compounds," *Phys. Rev. B* **42**, 4682 (1990).

J. M. Wills, Olle Eriksson, and A. M. Boring, "Theoretical Studies of the High Pressure Phases in Ce," *Phys. Rev. B* **67**, 2215 (1991).

J. M. Wills, Olle Eriksson, Per Söderlind, and A. M. Boring, "Trends of the Elastic Constants of Cubic Transition Metals," *Phys. Rev. Lett.* **68**, 2802 (1992).

J. M. Wills and Olle Eriksson, "Crystal-Structure Stabilities and Electronic Structure for the Light Actinides Th, Pa, and U," *Phys. Rev. B* **45** 13879 (1992-II).

W. G. Zittel, J. Meyer-ter-Vehn, J. C. Boettger, and S. B. Trickey, "Band-Reordering Effects in the Ultra-High Pressure Equation of State of Lithium," *J. Phys. F: Met Phys.* **15**, L247 (1985).

## Reports

- J. Abdallah, Jr., and W. F. Huebner, "QIKMIX: A Quick-Turnaround Computer Program for Computing Opacities of Mixtures," LANL report LA-7724-M (1979).
- J. Abdallah, Jr., "MIXB: A BCON Controller for Generating and Maintaining Sesame Library Files of Mixture Data," LANL report LA-8219-M (1980).
- J. Abdallah, Jr., G. I. Kerley, B. I. Bennett, J. D. Johnson, R. C. Albers, and W. F. Huebner "HYDSES: A Subroutine Package for Using Sesame in Hydrodynamic Codes," LANL report LA-8209 (1980).
- J. Abdallah, Jr., "User's Manual for CURVES," LANL report LA-8844-M (1981).
- J. Abdallah, Jr., "User's Manual for GRIZZLY" LANL report LA-10244-M (1984).
- R. C. Albers, "An Introduction to Two-Temperature Equations of State," LANL report LA-7934-MS (1979).
- R. C. Albers and J. E. Gubernatis, "Brillouin-Zone Integration Schemes: An Efficiency Study for the Phonon Frequency Moments of the Harmonic, Solid, One-Component Plasma," LANL report LA-8674-MS (1981).
- G. A. Baker, Jr., and J. D. Johnson, "Thomas-Fermi Equation of State-The Hot Curve," LANL report LA-11630-MS (1989).
- J. F. Barnes and S. P. Lyon, "SESAME Equation of State Number 7411,  $Al_2O_3$ ," LANL report LA-11058-MS (1987).
- J. F. Barnes and S. P. Lyon, "SESAME Equation of State Number 7100, Dry Sand," LANL report LA-11104-MS (1987).
- J. F. Barnes and S. P. Lyon, "SESAME Equation of State Number 7530, Basalt," LANL report LA-11253-MS (1988).
- B. I. Bennett, J. D. Johnson, G. I. Kerley, and G. T. Rood, "Recent Developments in the Sesame Equation of State Library," LANL report LA-7130 (1978).
- B. I. Bennett, "Melting Under Shock Compression," LANL report LA-8567-MS (1980).
- B. I. Bennett, "A Computationally Efficient Expression for the Zero-Temperature Isotherm in Equations of State," LANL report LA-8616-MS (1980).
- B. I. Bennett, "EOSSCAN: A Program to Display Equation of State Data," LANL report LA-8737-MS (1981).
- B. I. Bennett, "On Obtaining the Zero-Temperature Equation of State From Shock Data," LANL report LA-9890-MS (1983).
- B. I. Bennett, "An Equation of State for Titanium Dihydride," LANL report LA-9895-MS (1983).
- B. I. Bennett and D. A. Liberman, "INFERNO," LANL report LA-10309-M (1985).
- Equation-of-State and Opacity Group (T-4 Group), "An Invitation to Participate in the LASL Equation of State Library," N. G. Cooper, Ed., Los Alamos Scientific Laboratory brochure LASL-79-62 (1980).
- J. C. Boettger, "SESAME Equation of State Number 2293, Li," LANL report LA-11338-MS (1988).
- J. C. Boettger, "SESAME Equation of State Number 7486, Fused Quartz," LANL report LA-11488-MS (1989).
- J. C. Boettger, "Equation of State for a Polymer Composite, Phenolic Refrasil," LANL report LA-11512-MS (1989).

J. C. Boettger and S. P. Lyon, "Method of Obtaining SESAME Equations of State for Porous Materials: Application to Garnet Sand," LANL report LA-11726-MS (1990).

J. C. Boettger and J. M. Wills, "SESAME Equation of State Number 7611, Beryllium Oxide," LANL report LA-11768-MS (1990)

J. C. Boettger and S. P. Lyon, "New Multi-phase Equation of State for Polycrystalline Quartz," LANL report LA-11918-MS (1990).

J. C. Boettger, "SESAME Equation of State Number 7740: Polycarbonate," LANL report LA-12120-MS (1991).

J. C. Boettger and J. M. Wills, "Application of High Precision Band Structure Calculations to the Equation of State Number 7612," LANL report LA-12250-MS (1992).

F. Dowell and J. D. Johnson, "A Simple EOS for Polytetrafluoroethylene (Teflon)," LANL report LA-9439-MS (1982).

F. Dowell, "A Simple EOS for Branched (Low Density) Polyethylene," LANL report LA-9559-MS (1982).

F. Dowell, "A Simple EOS for Linear (High-Density) Polyethylene (Marlex)," LANL report LA-9564-MS (1982).

J. D. Johnson and B. I. Bennett, "An EOS for Carbon Phenolic," LANL report LA-9176-MS (1982).

J. D. Johnson, "Electron Model for Gaseous UO<sub>2</sub> EOS," in "Nuclear Reactor Safety Quarterly Progress Report, April 1-June 30, 1979," LANL report LA-7968-PR, NUREG/CR-0993 (1979).

J. D. Johnson and S. P. Lyon, "SES2D User's Manual," LANL report LA-9164-M (1982).

J. D. Johnson and S. P. Lyon, "EOS for Polycrystalline Quartz," LANL report LA-10391-MS (1985).

J. D. Johnson and S. P. Lyon, "New Equation of State for Eu, Gd, and Ho," LANL report LA-10439-MS (1985).

J. D. Johnson, "A Generic Model for the Ionic Contribution to the Equation of State," LANL report LA-UR-12003-MS (1991).

G. I. Kerley, "A New Equation of State for Sodium," in "Nuclear Reactor Safety Quarterly Progress Report, April 1-June 30, 1979," LANL report LA-7968-PR, NUREG/CR-0993 (1979).

G. I. Kerley and P. M. Henry, "Theoretical Equations of State for the Rare Gases," LANL report LA-8062 (1980).

G. I. Kerley "User's Manual for PANDA: A Computer Code for Calculating Equations of State," LANL report LA-8833-M (1981).

E. H. Lieb and D. A. Liberman, "Numerical Calculation of the Thomas-Fermion Weizsäcker Function for an Infinite Atom Without Electron Repulsion," LANL report LA-9186-MS (1982).

G. K. Straub and M. S. Shaw, "HYDROX - A One-Dimensional Lagrangian Hydrocode Including Reactive Flow and Dynamic Material Properties," LANL report LA-8642-M (1981).

G. K. Straub, "The Use of Molecular Dynamics for the Thermodynamic Properties of Simple and Transition Metals," LANL report LA-10959-MS (1987).

G. K. Straub, "Coulomb Electrostatic Contributions to the Energy, Pressure, Bulk Modulus, and Stress-Strain Coefficients in the Rock Salt Structure," LANL report LA-11232-MS (1988).

G. K. Straub, "Elastic Moduli of Copper: Electronic Structure Contributions from Pseudopotentials and Full-Potential Linear Muffin-Tin Orbital Bandstructure Calculations," LANL report LA-11522-MS (1989).

G. K. Straub, "Elastic Shear Modulus: Fits to Data and Extrapolation to Large Compressions and Negative Pressure," LANL report LA-11806-MS (1990).

## CURRENT LIST OF MATERIALS IN SESAME LIBRARY

Number	Material	Number	Material
1540	uranium	3210	indium
2020	beryllium	3280	gadolinium
2022	beryllium	3332	copper
2023	beryllium	3333	copper
2030	calcium	3334	copper
2110	europium	3510	cesium
2140	iron	3520	tantalum
2145	iron	3541	tungsten
2160	tin	3560	tungsten carbide
2290	lithium	3660	holmium
2291	lithium	3713	aluminum
2292	lithium	3715	aluminum
2293	lithium	3716	aluminum
2441	sodium	3717	aluminum
2448	sodium	3718	aluminum
2460	potassium	3719	aluminum
2550	vanadium	3730	platinum
2551	vanadium	3830	palladium
2680	cadmium	4100	brass
2700	gold	4270	stainless steel
2720	silver	4271	stainless steel
2740	niobium	5000	nitrogen
2810	rubidium	5001	nitrogen
2860	magnesium	5010	oxygen
2961	titanium alloy	5011	oxygen
2962	titanium alloy	5030	dry air
2980	molybdenum	5171	argon
2981	molybdenum	5172	argon
2982	molybdenum	5180	krypton
2983	molybdenum	5181	krypton
3050	rhodium	5190	xenon
3070	chromium	5210	carbon dioxide
3100	nickel	5250	hydrogen
3101	nickel	5251	hydrogen
3120	cobalt	5263	deuterium
3140	zinc	5271	d-t mixture
3180	zirconium	5272	d-t mixture
3200	lead	5280	ross-aller solar mix



<b>Number</b>	<b>Material</b>	<b>Number</b>	<b>Material</b>
5300	sr-xe mixture	7331	calcite
5410	neon	7371	lithium hydride
5411	neon	7380	quartz
5500	methane	7381	quartz
5501	methane	7383	polycrystal quartz
5502	methane	7385	polycrystal quartz
5520	ammonia	7386	fused quartz
5530	normal butane	7387	fused quartz
5540	isobutane	7390	westerly granite
5760	helium	7391	westerly granite
5761	helium	7410	alumina
5762	helium	7411	alumina
7030	leaded glass	7432	uranium dioxide
7081	boron carbide	7440	hematite
7100	dry sand	7450	calcium oxide
7102	dry clay	7460	periclase
7111	nevada alluvium	7470	titanium dioxide
7112	nevada alluvium	7480	niobium tritide
7120	saturated tuff	7510	dolomite
7121	saturated tuff	7520	mica
7122	saturated tuff	7521	muscovite (mica)
7130	limestone	7530	basalt
7150	water	7541	carbon phenolic
7152	water	7552	carbon phenolic
7153	water	7550	mylar
7154	water	7560	polyurethane
7160	deutero-polyethylene	7561	polyurethane
7171	polyethylene (branched)	7570	phenolic
7180	polyethylene (marlex)	7580	phenolic refrasil
7190	teflon	7590	polystyrene
7230	polytetra-deutero- ethylene	7591	polystyrene
7244	lithium(n)-deuteride	7592	polystyrene
7245	lithium(6)-deuteride	7601	epoxy
7252	lithia-boria glass	7602	epoxy
7270	lithium fluoride	7603	epoxy
7281	salt	7610	beryllium oxide
7282	salt	7611	beryllium oxide
7283	salt	7612	beryllium oxide
7330	calcium carbonate	7660	perphenylene sulfide
		7740	polycarbonate

<b>Number</b>	<b>Material</b>
7741	polycarbonate (lexan)
7750	lucite
7760	garnet
7761	garnet sand
7770	parylene
7771	parylene
7830	diamond
7831	carbon liquid
7832	carbon (graphite)
7833	carbon (graphite)
7930	sylgard
7931	sylgard 184
8010	boron loaded silicone
8020	polyetheretherketone (peek)
8200	pbx-9502

## MELT AND SHEAR TABLES

Number	Material	Number	Material
31540	uranium	37030	leaded glass
32023	beryllium	37112	nevada alluvium
32030	calcium	37270	lithium fluoride
32140	iron	37387	fused quartz
32160	tin	37470	titanium dioxide
32292	lithium	37480	niobium tritide
32293	lithium	37603	epoxy
32441	sodium	37741	polycarbonate (lexan)
32460	potassium	37770	parylene
32551	vanadium	37771	parylene
32680	cadmium	37832	carbon
32700	gold	37833	carbon
32720	silver		
32740	niobium		
32810	rubidium		
32860	magnesium		
32980	molybdenum		
32983	molybdenum		
33050	rhodium		
33070	chromium		
33100	nickel		
33101	nickel		
33120	cobalt		
33140	zinc		
33180	zirconium		
33200	lead		
33210	indium		
33330	copper		
33332	copper		
33510	cesium		
33520	tantalum		
33540	tungsten		
33541	tungsten		
33710	aluminum		
33717	aluminum		
33830	palladium		
34271	stainless steel 347		