Shock Wave Data for Minerals

Thomas J. Ahrens and Mary L. Johnson

1. INTRODUCTION

Shock compression of the materials of planetary interiors yields data, which upon comparison with density-pressure and density-sound velocity profiles of both terrestrial planetary mantles and cores [4,5,94], as well as density profiles for the interior of the major planets [148], constrain internal composition and temperature. Other important applications of shock wave data and related properties are found in the impact mechanics of terrestrial planets and the solid satellites of the terrestrial and major planets. Significant processes which can, or have been, studied using shock wave data include: (1) the formation of planetary metallic cores during accretion [169,192], and (2) the production of a shock-melted "magma ocean" and concurrent impact volatilization versus retention of volatiles during accretion [1]. Also of interest are the shock-induced chemical reactions between meteoritic components (e.g. H2O and Fe: [111]). The formation of primitive atmospheres, for example, containing a large fraction of H2O and CO2 is also addressable using shock wave and other thermodynamic data for volatile-bearing minerals (e.g. [110,112]). A related application of both shock

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compression and isentropic release data for minerals [13,14] is in the mechanics of both the continued bombardment and hence cratering on planetary objects through geologic time [170], as well as the effects of giant impacts on the Earth [183,185]. Finally, recovery and characterization of shock-compressed materials have provided important insights into the nature of shock deformation mechanisms and, in some cases, provided physical data on the nature of either shock-induced phase changes or phase changes which occur upon isentropic release from the high-pressure shock state (e.g., melting) [193,194].

As indicated for the data summary of Table 1, a very large data set exists describing the Hugoniot equation of state of minerals. Whereas some earlier summaries have provided raw shock data [47,121,213], the present summary provides fits to shock wave data. Earlier summaries providing fits to data are given by Al'tshuler et al. [24] and Trunin [203].

Hugoniot data specify the locus of pressure-density (or specific volume) states which can be achieved by a mineral from some initial state with a specified initial density. An analogous summary for rocks, usually described as a mixture of minerals are given in Chapter 3-4.

Three pressure units are commonly in use in the shock wave literature: kilobar (kbar), gigapascal (GPa), and megabar (Mbar). These are equal to $10^9$, $10^{10}$, and $10^{12}$ dyne/cm$^2$, respectively, or $10^8$, $10^9$, and $10^{11}$ pascals in SI units.

2. SHOCK WAVE EQUATION OF STATE

The propagation of a shock wave from a detonating explosive or the shock wave induced upon impact of a flyer plate accelerated, via explosives or with a gun, result in nearly steady waves in materials. For steady waves a shock velocity $U_s$ with respect to the laboratory frame can
be defined. Conservation of mass, momentum, and energy across a shock front can then be expressed as

\begin{align*}
\rho_1 &= \rho_0 \frac{(U_3-u_0)}{(U_3-u_1)} \quad (1) \\
P_1 - P_0 &= \rho_0 (u_1-u_0) \frac{(U_3-u_0)}{(U_3-u_1)} \quad (2) \\
E_1 - E_0 &= \frac{(P_1 + P_0)(1/\rho_0 - 1/\rho_1)}{2} = \frac{1}{2} (u_1 - u_0)^2 \quad (3)
\end{align*}

where \(\rho\), \(u\), \(P\), and \(E\) are density, particle velocity, shock pressure, and internal energy per unit mass and, as indicated in Fig. 1, the subscripts 0 and 1 refer to the state in front of and behind the shock front, respectively. In Table 1, shock velocity and particle velocity are designated as \(U_3\) and \(U_p\). Equations (1)-(3) are often called the Rankine-Hugoniot equations. It should be understood that in this section pressure is used in place of stress in the indicated wave propagation direction. In actuality, stress in the wave propagation direction is specified by Eq. (2). A detailed derivation of Eqs. (1), (2), and (3) is given in Duvall and Fowles [70]. Equation (3) also indicates that the material achieves an increase in internal energy (per unit mass) which is exactly equal to the kinetic energy per unit mass.

In the simplest case, when a single shock state is achieved via a shock front, the Rankine-Hugoniot equations involve six variables \((U_3, u_1, \rho_0, P_1, E_1 - E_0\), and \(P_1\); thus, measuring three, usually \(U_3\), \(u_1\), and \(\rho_0\) determines the shock state variables \(P_1\), \(E_1 - E_0\) and \(P_1\).

The key assumption underpinning the validity of Eqs. (1)-(3) is that the shock wave is steady, so that the rise time \(t_s\) is short compared to the characteristic time for which the high pressure, density, etc. are constant (see Fig. 1). Upon driving a shock of pressure \(P_1\) into a material, a final shock state is achieved which is described by Eqs. (1)-(3). This shock state is shown in Fig. 2, in relation to other thermodynamic paths, in the pressure-volume plane. Here \(V_0 = 1/\rho_0\) and \(V = 1/\rho\). In the case of the isotherm and isentrope, it is possible to follow, as a thermodynamic path, the actual isothermal or isentropic curve to achieve a
state on the isotherm or isentrope. A shock, or Hugoniot, state is different, however. The Hugoniot state \((P_1, V_1)\) is achieved via a shock front. The initial and final states are connected by a straight line called a Rayleigh line (Fig. 2). Thus successive states along the Hugoniot curve cannot be achieved, one from another, by a shock process. The Hugoniot curve itself then just represents the locus of final shock states corresponding to a given initial state.

It has long been recognized that the kinematic parameters measured in shock wave experiments \(U_s\) and \(U_p\) can empirically be described in regions where a substantial phase change in the material does not occur as:

\[
U_s = C_0 + S U_p
\]  
(4)

As further discussed in several review articles on shock compression [22,59,136], and a recent book [40], Hugoniot data for minerals and other condensed media may be described over varying ranges of pressure and density in terms of a linear relation of shock and particle velocity in Table 1. This table was assembled using the Microsoft Excel, version 3.0, (Redmond, WA 1993) program and the least-square fits to the shock wave data with standard errors were derived by using the LINEST function. The equations employed for line slopes and intercepts are identical to those given in Bevington [46] (Eq. 6-9, p. 104; Eq. 6-21, p. 114 for errors in slopes; and Eq. 6-22, p. 114 for errors in intercepts).

The \(U_s-U_p\) data for a wide range of minerals are given in Table 1. Here \(C_0\) is the shock velocity at infinitesimally small particle velocity, or the ambient pressure bulk sound velocity which is given by

\[
C_0 = \sqrt{K_s/\rho_0},
\]  
(5)

where \(K_s\) is the isentropic bulk modulus.
\( K_s = -V \frac{dP}{dV} \) is in the absence of strength effect (see Sect. 3). Upon substituting Eq. 4 into Eq. 2, and denoting the shock pressure as \( P_H \), this is given by:

\[
P_H = \rho_0 U_p (C_0 + S U_p)
\]  

(6)

Thus, from the form of Eq. 6, shock pressure is given as the sum of a linear and quadratic term in particle velocity, based on the data of Table 1. A pressure-volume relation can be obtained by combining Eq. 6 with Eq. 1 to yield:

\[
P_H = \rho_0 C_0^2 \eta / (1 - S \eta)^2
\]  

(7)

where

\[
\eta = 1 - V/V_0 = U_p / U_S.
\]  

(8)

Eq. 7 is often called the "shock wave equation of state" since it defines a curve in the pressure-volume plane.

The isentropic pressure can be written (e.g. [93,98,171]) by an expression analogous to Eq. 7 as a series

\[
P_S = \rho_0 C_0^2 (\eta + 2S \eta^2 +...),
\]  

(9)

which upon differentiation yield the isentropic bulk modulus

\[
K_s = \rho_0 C_0^2 (1 + (4S - 1) \eta +...)
\]  

(10)

The analogous bulk modulus along the Hugoniot is:

\[
K_H = -V \frac{\partial P}{\partial V}_H.
\]  

(11)

The isentrope and the Hugoniot and isentropic bulk modulus are related via:

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Here we assume a volume dependence of the Gruneisen parameter

\[ \gamma = V \frac{\partial P}{\partial E}_V = \gamma_0 \left( \frac{V}{V_0} \right)^q, \]  

(13)

where

\[ q = \frac{\partial \ln \gamma}{\partial \ln V} \quad \text{and} \quad q' = \frac{\partial \ln q}{\partial \ln V} \]  

(14)

\[ \gamma_0 \] is the Gruneisen parameter under standard pressure and temperatures and is given by

\[ \gamma_0 = \alpha K_T V_0/C_V = \alpha K_s V_0/C_p, \]  

(15)

where \( \alpha \) is the thermal expansion coefficient, \( K_T \) is the isothermal bulk modulus and \( C_p \) and \( C_V \) are the specific heat at constant pressure and volume. We note that the \( P_s \) and \( P_H \) can be related by assuming the Mie-Grüneisen relation

\[ P_H - P_s = \frac{\gamma}{V} (E_H - E_s), \]  

(16)

if \( \gamma \) is independent of temperature, where \( E_H = E_1 - E_0 \) is given by Eq. 3 and \( E_s \) is given by

\[ E_s = - \int_{V_0}^{V} P_s dV. \]  

(17)

Because the Grüneisen ratio relates the isentropic pressure, \( P_s \), and bulk modulus, \( K_s \), to the Hugoniot pressure, \( P_H \), and Hugoniot bulk modulus, \( K_H \), it is a key equation of state parameter.

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The shock-velocity particle relation of Table 1 can be used to calculate the shock pressure when two objects impact. If (A) the flyer plate and (B) the target are known and expressed in the form of Eq. (7), the particle velocity $u_1$ and pressure $P_1$ of the shock state produced upon impact of a flyer plate at velocity $u_{fp}$ on a stationary target may be calculated from the solution of the equation equating the shock pressures in the flyer and driver plate:

$$
\rho_o A (u_{fp} - u_1)(C_o A + S_A (u_{fp} - u_1)) = \\
\rho_o B u_1 (C_o B + S_B u_1).
$$

That is,

$$
u_1 = \frac{-b - \sqrt{b^2 - 4ac}}{2a},
$$

where

$$a = S_A \rho_o A - \rho_o B S_B,$$

$$b = C_o A \rho_o A - 2S_A \rho_o A u_{fp} - \rho_o B C_o B,$$

and

$$c = u_{fp} (C_o A \rho_o A + S_A \rho_o A u_{fp}).$$

3. SHOCK-INDUCED DYNAMIC YIELDING AND PHASE TRANSITIONS

Both dynamic yielding and phase transitions give rise to multiple shock wave profiles when pressure or particle velocity versus time is recorded. Virtually all nonporous minerals and rocks in which dynamic compression has been studied demonstrate phenomenon related to dynamic yielding, in which materials transform from finite elastic strain states to states in which irreversible deformation has occurred. Moreover, most minerals and a large number of

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compounds, elements, and organic materials demonstrate shock-induced phase changes.

The dynamic yield point under shock compression, the Hugoniot elastic limit, or HEL, is defined as the maximum shock pressure a material may be subjected to without permanent, massive, microscopic rearrangement taking place at the shock front. As shown in Fig. 3a, the shock velocity of the HEL state remains nearly constant and for non-porous media is usually equal to the longitudinal elastic wave velocity. Viscoelastic polymeric media generally do not display the HEL phenomenon. We denote five regimes in Fig. 3 for the case of dynamic yielding and phase transition and the available shock wave data are separately fit to linear relations in these regimes in Table 1. For some minerals there are more than four regimes indicated, for reasons such as crystallographic control of compression at low pressures (such as Oa, Ob for quartz), and for more than one high-pressure state (such as 4a, 4b, and 4c for halite).

The crystallographic or atomistic level nature of shock-induced phase changes varies from simple average coordination changes observed in various liquids, ionization and debonding in non-metallic fluids, electronic transitions in metal and non-metals, changes in crystal structure in solid materials, and transition from the solid to the fluid state.

In the case of a phase change, the pressure along the isentrope $P_s$ at the volume $V_1$ corresponding to a Hugoniot state $(P_1, V_1)$ is given by

$$\frac{P_1}{2} (V_{oo} - V_1) = - \int \frac{V_1}{V_0} P dV + \frac{V_1}{V_0} (P_1 - P_s) + ETR$$

(23)

where the left-hand side is the Rankine-Hugoniot energy, and the first and second terms on the right represent the gain in the internal energy along the paths 1 and 2 of Fig. 2. Here $V_{oo}$ is the specific volume of the initial material and $V_0$ the specific volume of the shock-induced high-pressure phase, or the intrinsic volume of the sample if the

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initial state is distended. Also $E_{TR}$ is the energy of transition to the high-pressure phase at STP. In the case of no phase change, $E_{TR} = 0$. For zero initial porosity $V_{oo} = V_0$. The unknown parameter in Eq. 23 is $P_s$, which is implicit in the first integral term on the right-hand side and explicit in the second term. The second term is obtained by using the definition of the Gruneisen parameter (Eq. 13) to calculate the change in energy associated with the pressure difference $(P_1-P_s)$ at constant volume.

4. SHOCK TEMPERATURES

For many condensed media, the Mie-Gruneisen equation of state, based on a finite-difference formulation of the Gruneisen parameter (Eq. 16), can be used to describe shock and postshock temperatures. The temperature along the isentrope [224] is given by

$$T_s = T_i \exp \left[ - \int \frac{V_b}{V_a} \left( \frac{\gamma}{\gamma} \right) dV \right]$$

(24)

where $T_i$ is the initial temperature. For the principal isentrope centered at room temperature, $T_i = T_0$, $V_a = V_o$, initial volume, and $V_b = V$, compressed volume. For the calculation of postshock temperatures $T_i = T_H$, the Hugoniot temperature, $V_a = V_H$, the volume of the shock state, and $V_b = V_{oo}$, the postshock volume corresponding to the postshock temperature. For shock compression to a volume $V$, $P_s$ is first obtained by using Eq. 23; then $T_s$, the isentropic compression temperature at volume $V$, may be calculated by using Eq. 24. Finally, using Eq. 16, the shock temperature $T_H$ is given by

$$\frac{V}{\gamma} \left( P_H - P_s \right) = \int T_s dT$$

(25)

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It is useful to carry out both postshock and shock temperature measurements as they provide complementary information for the thermal equation of state, that is, $\gamma$ as well as $C_V$. Minerals for which shock temperatures have been (usually via radiative techniques) are so indicated in Table 1.

In the case of molecular fluids such as water, a formulation based on the near constancy of $C_p$ at constant pressure is used [41,167].

Although there have been few data collected, postshock temperatures are very sensitive to the models which specify $\gamma$ and its volume dependence, in the case of the Gruneisen equation of state [49,164,165]. In contrast, the absolute values of shock temperatures are sensitive to the phase transition energy $E_{TR}$ of Eq. 23, whereas the slope of the $T_H$ vs. pressure curve is sensitive to the specific heat.

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FIGURE CAPTIONS

FIG. 1. Profile of a steady shock wave, rise time $\tau_s$, imparting a particle velocity $u_1$ pressure $P_1$, and internal energy density $E_1$, propagating with velocity $U_s$ into material that is at rest at density $\rho_0$ and internal energy density $E_0$.

FIG. 2. Pressure-volume compression curves. For isentrope and isotherm, the thermodynamic path coincides with the locus of states, whereas for shock, the thermodynamic path is a straight line to point $P_1,V_1$, on the Hugoniot curve, which is the locus of shock states.

FIG. 3. Sketch of shock velocity-particle relation (a) and corresponding pressure-volume Hugoniot curves (b) for a mineral which undergoes dynamic yielding and a phase change.

0: compression up to the Hugoniot Elastic Limit (HEL)
1: transition via dynamic yielding to a quasi-hydrostatic state
2: low pressure state
3: mixed region
4: high pressure state
<table>
<thead>
<tr>
<th>Mineral</th>
<th>Formula</th>
<th>Sample Density (Mg/m³)</th>
<th>C₀ (km/sec)</th>
<th>error ΔC₀ (km/sec)</th>
<th>S</th>
<th>error ΔS (km/sec)</th>
<th>U_p lower (km/sec)</th>
<th>U_p upper (km/sec)</th>
<th>Phase</th>
<th>No. of Data</th>
<th>References / Temp. Refs.</th>
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<td>5.788</td>
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## TABLE 1. Shock Wave Equation of State of Minerals and Related Materials of the Solar System

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<thead>
<tr>
<th>Mineral</th>
<th>Formula</th>
<th>Sample Density (Mg/m³)</th>
<th>C₀ (km/sec)</th>
<th>error ΔC₀ (km/sec)</th>
<th>S</th>
<th>error ΔS (km/sec)</th>
<th>lower Uₚ (km/sec)</th>
<th>upper Uₚ (km/sec)</th>
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<th>References / Temp. Refs.</th>
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May 9, 1994
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May 9, 1994
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TABLE 1. Shock Wave Equation of State of Minerals and Related Materials of the Solar System

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**Carbides:**

| Moissanite SiC | 2.333 | 2.3 | 0.3 | 1.84 | 0.12 | 2.048 | 3.444 | 4 | 10 | [121,127,136] |
| Moissanite SiC | 3.029 | 8.4 | 0.6 | 0.3 | 0.3 | 1.535 | 2.112 | 3 | 3 | [121] |
| Moissanite SiC | 3.122 | 8.0 | -- | 6.0 | -- | 0.00 | 0.464 | 1 | 2 | [121,127,136] |
| Moissanite SiC | 10.29 | 10.29 | 0.13 | -0.38 | 0.10 | 0.674 | 1.678 | 3 | 9 | [121,127,136] |
| Moissanite SiC | 7.84 | 7.84 | 0.11 | 1.03 | 0.05 | 1.678 | 2.912 | 4 | 10 | [121,127,136] |

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## TABLE 1. Shock Wave Equation of State of Minerals and Related Materials of the Solar System

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<tr>
<th>Mineral</th>
<th>Formula</th>
<th>Sample Density (Mg/m³)</th>
<th>Error ΔC₀ (km/sec)</th>
<th>S Error ΔS (km/sec)</th>
<th>Lower U₀ (km/sec)</th>
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<th>No. of Data</th>
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# TABLE 1. Shock Wave Equation of State of Minerals and Related Materials of the Solar System

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### TABLE 1. Shock Wave Equation of State of Minerals and Related Materials of the Solar System

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<th>Mineral</th>
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### TABLE 1. Shock Wave Equation of State of Minerals and Related Materials of the Solar System

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### TABLE 1. Shock Wave Equation of State of Minerals and Related Materials of the Solar System

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## TABLE 1. Shock Wave Equation of State of Minerals and Related Materials of the Solar System

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TABLE 1. Shock Wave Equation of State of Minerals and Related Materials of the Solar System

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### TABLE 1. Shock Wave Equation of State of Minerals and Related Materials of the Solar System

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<th>ΔC₀ (km/sec)</th>
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TABLE 1. Shock Wave Equation of State of Minerals and Related Materials of the Solar System

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Pyroxenes:

| Enstatite  | Mg₂-Si₂O₆       | 2.714                  | 2.70        | 0.11         | 1.31 | 0.04| 1.901            | 3.258            | 2     | 5           | [47,121,217]             |
| Enstatite  | Mg₂-Si₂O₆       | 2.814                  | 2.74        | 0.14         | 2.04 | 0.09| 0.746            | 1.956            | 2     | 5           | [121,127]                |
| Enstatite  | Mg₂-Si₂O₆       | 3.067                  | 8.11        | 0.18         | -1.5 | 0.4 | 0.224            | 0.60             | 1     | 6           | [8,121,127,231] / [117,165] |
| Diopside   | CaMgSi₂O₆       | 3.264                  | 4.9         | --           | 8.4  | -- | 0.201            | 0.289            | 1     | 2           | [18,196,213] / [198]     |

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TABLE 1. Shock Wave Equation of State of Minerals and Related Materials of the Solar System

<table>
<thead>
<tr>
<th>Mineral</th>
<th>Formula</th>
<th>Sample Density (Mg/m$^3$)</th>
<th>$C_0$ (km/sec)</th>
<th>$\Delta C_0$ (km/sec)</th>
<th>$S$</th>
<th>$\Delta S$</th>
<th>lower $U_p$ (km/sec)</th>
<th>upper $U_p$ (km/sec)</th>
<th>Phase$^a$</th>
<th>No. of Data</th>
<th>References / Temp. Refs.</th>
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<td>$(\text{NaAlSi}_3\text{O}<em>8)</em>{75}(\text{CaAl}_2\text{Si}_2\text{O}<em>8)</em>{19.5}$</td>
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TABLE 1. Shock Wave Equation of State of Minerals and Related Materials of the Solar System

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<th>Formula</th>
<th>Sample Density (Mg/m³)</th>
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<th>ΔC₀ (km/sec)</th>
<th>S</th>
<th>error ΔS (km/sec)</th>
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May 9, 1994
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May 9, 1994
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### TABLE 1. Shock Wave Equation of State of Minerals and Related Materials of the Solar System

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<th>ΔC₀ (km/sec)</th>
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Notes:

*Phases: 1) Elastic shock; 2) Low pressure phase; 3) Mixed region; 4) High pressure phase.

a Starting temperature 5K
b Starting temperature 20K
c Starting temperature 75-86K
d Starting temperature 111K
e Starting temperature 122K
f Starting temperature 148K; compressed gas
g Starting temperature 165K
h Starting temperature 196K

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TABLE 1. Shock Wave Equation of State of Minerals and Related Materials of the Solar System

<table>
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<tr>
<th>Mineral</th>
<th>Formula</th>
<th>Sample Density (Mg/m³)</th>
<th>C₀ (km/sec)</th>
<th>ΔC₀ (km/sec)</th>
<th>S</th>
<th>ΔS</th>
<th>lower Uᵣ (km/sec)</th>
<th>upper Uᵣ (km/sec)</th>
<th>Phase*</th>
<th>No. of Data</th>
<th>References / Temp. Refs.</th>
</tr>
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</table>

i Starting temperature 203-230K
j Starting temperature 258-263K
k Starting temperature 273-298K
l Starting temperature 300K; compressed gas
m Starting temperature 1673K
n Starting temperature 1773K
o Starting temperature 1923 K
p 5% cobalt
q raw data not provided
r with impurities
s composition in weight percent oxides

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