NORTH ATLANTIC TREATY ORGANIZATION
ORGANISATION DU TRAITE DE L'ATLANTIQUE NORD

MILITARY AGENCY FOR STANDARDIZATION (MAS)
BUREAU MILITAIRE DE STANDARDISATION (BMS)
1110 BRUSSELS

MAS/204-LAND/4400
3 June 1993

To : See MAS Distribution List No. 2

Subject : STANAG 4400 LAND (EDITION 1) - DERIVATION OF THERMOCHEMICAL VALUES FOR INTERIOR BALLISTIC CALCULATION

Reference : AC/225-D/1245 dated 31 August 1992

Enclosure : STANAG 4400 (Edition 1)

1. The enclosed NATO Standardization Agreement which has been ratified by nations as reflected in page iii is promulgated herewith.

2. The reference listed above is to be destroyed in accordance with local document destruction procedures.

3. AAP-4 should be amended to reflect the latest status of the STANAG.

ACTION BY NATIONAL STAFFS

4. National staffs are requested to examine page iii of the STANAG and if they have not already done so, to advise the Defence Support Division, IS, through their national delegation as appropriate of their intention regarding its ratification and implementation.

E. STAI
Major-General, NOAF
Chairman, MAS

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STANAG 4400
(Edition 1)

NORTH ATLANTIC TREATY ORGANIZATION
(N A T O)

MILITARY AGENCY FOR STANDARDIZATION
(M A S)

STANDARDIZATION AGREEMENT

SUBJECT : DERIVATION OF THERMOCHEMICAL VALUES FOR INTERIOR BALLISTIC CALCULATION

Promulgated on 3 June 1993

E. STAI
Major-General, NOAF
Chairman, MAS

RECORD OF AMENDMENTS

No.	Reference/date of amendment	Date entered	Signature

EXPLANATORY NOTES

AGREEMENT

1. This NATO Standardization Agreement (STANAG) is promulgated by the Chairman MAS under the authority vested in him by the NATO Military Committee.

2. No departure may be made from the agreement without consultation with the tasking authority. Nations may propose changes at any time to the tasking authority where they will be processed in the same manner as the original agreement.

3. Ratifying nations have agreed that national orders, manuals and instructions implementing this STANAG will include a reference to the STANAG number for purposes of identification.

DEFINITIONS

4. Ratification is "The declaration by which a nation formally accepts the content of this Standardization Agreement".

5. Implementation is "The fulfilment by a nation of its obligations under this Standardization Agreement".

6. Reservation is "The stated qualification by a nation which describes that part of this Standardization Agreement which it cannot implement or can implement only with limitations".

RATIFICATION, IMPLEMENTATION AND RESERVATIONS

7. Page iii gives the details of ratification and implementation of this agreement. If no details are shown, it signifies that the nation has not yet notified the tasking authority of its intentions. Page iv (and subsequent) gives details of reservations and proprietary rights that have been stated.

STANAG 4400
(Edition 1)

NAVY/ARMY

NATO STANDARDIZATION AGREEMENT
(STANAG)

DERIVATION OF THERMOCHEMICAL VALUES FOR INTERIOR BALLISTIC CALCULATIONS

Annexes:
- A - Relations and Definitions of Thermochemical Properties
- B - Glossary of Terms
- C - Calculation of the Ratio of "Frozen" Specific Heats
- D - Method of Calculation of Second and Third Virial Coefficients
- E - Coefficients of Heat Capacity, Enthalpy, and Entropy
- F - Atomic Weights and Constants
- G - Table of Formulas and Enthalpies of Propellant Ingredients
- H - Summary of Propellant Characteristics
- I - Selected Bibliography

Related Documents:
- STANAG 4367 - Thermodynamic Interior Ballistic Model with Global Parameters
- STANAG 4117 - Stability Test Procedures and Requirements for Propellants Stabilized with Diphenylamine, Ethyl Centralite or a Mixture of Both
- STANAG 4115 - Definition and Determination of Ballistic Properties of Gun Propellants
- Annex I

AIM

1. The aim of this agreement is to standardize the determination of thermochemical values for use in interior ballistic calculations.

AGREEMENT

2. Participating nations agree to use the methodology described in the Annexes to determine thermochemical values for use in the interior ballistic simulation model described in STANAG 4367.

DEFINITIONS

3. The definitions used for the purpose of this STANAG are given in Annex B.

GENERAL

4. This document also provides the agreed upon data to be used in the model. These data are independent of the model chosen for the calculation.

IMPLEMENTATION OF THE AGREEMENT

5. This STANAG is implemented when a nation has issued instructions to the agencies concerned to use the Thermochemical Values for Interior Ballistic Calculations as detailed in this agreement.

RELATIONS AND DEFINITIONS OF THERMOCHEMICAL PROPERTIES

1. Many different approaches to the calculation of thermochemical values for use in interior ballistic codes could be followed. In order to assure a unified approach, the participating nations have agreed on the following assumptions:

   a. The products of combustion are in thermochemical equilibrium and there is no heat loss during combustion.

   b. The virial equation of state, truncated after the third term, or any equation which is equivalent to the third order, is used.

   c. The thermochemical equilibrium is obtained by minimizing the free energy, subject to appropriate restrictions (eg fixed volume and fixed energy).

   d. The propellant compositions contain the following elements at a minimum:

      C, H, O, N, S, K, Al, Na, Ba, Mg, F and Pb.

   e. The ratio of the "frozen" specific heat capacities is calculated. The method is given in Annex C.

2. The truncated virial equation of state is

$$PV = nRT\ [1+\frac{nB}{V}+(\frac{n}{V})^2 C]$$

where B and C are the second and third virial coefficients. A list of symbols used in this Annex is given at the end of this Annex. The second and third virial coefficients are calculated by the method given in Annex D.

3. Minimization of Gibbs Energy

For a mixture of m species, the Gibbs energy per kilogram of mixture, g, is given by

$$g = \sum_{j=1}^{m} \mu_j\, n_j$$

where the chemical potential per mole of species j is defined as

$$\mu_j = \left(\frac{\partial g}{\partial n_j}\right)_{T,\ P,\ n_{i \neq j}}$$

The condition for chemical equilibrium is the minimization of energy. This minimization is subject to the following mass balance constraint

$$b_i - b_i^o = 0 \qquad i = 1, \ldots, \ell$$

where

$$b_i = \sum_{j=1}^{m} a_{ij} n_j \qquad i = 1, \ldots, \ell$$

where the stoichiometric coefficients a_{ij} are the number of atoms of element i per mole of species j, and b_i^o is the assigned amount of atoms of element i per kilogram of total reactants. Defining a term G to be

$$G = g + \sum_{i=1}^{\ell} \lambda_i \left(\sum_{j=1}^{m} a_{ij} n_j - b_i^o\right)$$

where λ_i are Lagrangian multipliers, the condition for equilibrium becomes

$$\delta G = \sum_{j=1}^{m} \left(\mu_j + \sum_{i=1}^{\ell} \lambda_i a_{ij}\right) \delta n_j + \sum_{i=1}^{\ell} \left(b_i - b_i^o\right) \delta \lambda_i = 0$$

4. Minimization of Helmoltz Energy

The equations here are similar to those presented in the previous section. The two free energies have the following thermodynamic relationship:

$$f = g - PV$$

where f is the Helmholtz energy per kilogram of mixture, and g is given in section 3, that is

$$f = \sum_{j=1}^{m} \mu_j n_j - PV$$

The chemical potential μ_i can be expressed as the following thermodynamic derivative

$$\mu_j = \left(\frac{\partial f}{\partial n_j}\right)_{T,\ V,\ n_{i \neq j}}$$

If $$F = f + \sum_{i=1}^{\ell} \lambda_i \ (b_i - b_i^{\circ})$$

the condition for equilibrium based on the minimization of the Helmholtz energy subject to mass balance constraints is

$$\delta F = \sum_{j=1}^{m} \left(\mu_j + \sum_{i=1}^{\ell} \lambda_i a_{ij}\right) \delta n_j + \sum_{i=1}^{\ell} (b_i - b_i^{\circ}) \ \delta \lambda_i = 0$$

5. Thermodynamic Data

For each reaction species, the thermodynamic functions specific heat, enthalpy, and entropy as functions of temperature are given in the form of least squares coefficients as follows:

$$C_p^{\circ} = R \ [a_0 + a_1 T + a_2 T^2 + a_3 T^3 + a_4 T^4]$$

$$H_T^{\circ} = RT \ \left[a_0 + \frac{a_1}{2} T + \frac{a_2}{3} T^2 + \frac{a_3}{4} T^3 + \frac{a_4}{5} T^4 + \frac{a_5}{T}\right]$$

$$S_T^{\circ} = R \ [a_0 \ln T + a_1 T + \frac{a_2}{2} T^2 + \frac{a_3}{3} T^3 + \frac{a_4}{4} T^4 + a_6]$$

and

$$H_T^{\circ} = (\Delta H_f)_{298.15} + \int_{298.15}^{T} C_p^{\circ} dT$$

$$S_T^{\circ} = S_{298.15}^{\circ} + \int_{298.15}^{T} C_p^{\circ} d(\ell nT)$$

For each species, two sets of coefficients are included for two adjacent temperature intervals, 300 to 1000K and 1000 to 5000K. The data have been constrained to be equal at 1000K. Examples of the coefficients are given in Annex E. The standard state is defined as the stable form of a pure element at a pressure of 0.1MPa and a temperature of 298.15K for which $\Delta H_f = H_f^{\circ} = 0$. The temperature is obtained by equalising the internal energy of the combustion products with the internal energy of the propellant.

Annex F contains the atomic weights and constants, Annex G contains a table of formulas and enthalpies of propellant ingredients. A format for summarising propellant characteristics is given in Annex H.

The data given in Annex E-G are only examples of the data required because they are always subject to revision. France is responsible for maintaining and updating a reference database which is available to all nations.

6. Covolume, η, is defined as $V-f_p/P$, where f_p is the propellant force and is equal to $(n\ R\ T_f)$. The covolume is calculated from the second and third Virial coefficients, B and C, by the following equation

$$\eta = \frac{nBV^2+n^2CV}{V^2+nBV+n^2C}$$

LIST OF SYMBOLS

Symbol	Definition	SI Units
a_{ij}	Stoichiometric coefficients, number of atoms of element i per mole of species j	-
a_i (i=o to 6)	Least squares coefficients	Various
b_i	Amount of atoms of element i per kilogram of mixture	mol/kg
b_i^o	Assigned amount of atoms of element i per kilogram of total reactants	mol/kg
B	Second virial coefficient	m^3/mol
C	Third virial coefficient	$m^6/(mol^2)$
C_p^o	Standard state molar heat capacity at constant pressure	J/(mol-K)
f	Helmholtz specific energy of mixture	J/kg
f_p	Propellant force	J/kg
F	Helmholtz specific energy with constraints	J/kg
g	Gibbs specific energy of mixture	J/kg
G	Gibbs specific energy with constraints	J/kg
H_T^o	Standard state molar enthalpy	J/mol
n	Number of moles of gas per kilogram	mol/kg
n_j	Amount of moles of species j per kilogram of mixture	mol/kg
P	Pressure	Pa
R	Molar gas constant	J/(mol-K)
S_T^o	Standard state molar entropy	J/(mol-K)

T	Thermodynamic temperature	K
T_f	Adiabatic flame temperature	K
V	Specific volume	m^3/kg
ΔH_f	Enthalpy of formation	J/mol
μ_j	Chemical potential of species j	J/mol
η	Propellant covolume	m^3/kg
λ_i	Lagrangian multiplier	J/mol

GLOSSARY OF TERMS

1. Propellant Force, f_p

This is a quantity used by interior ballisticians. It represents the work capacity of the propellant and is proportional to the energy released by a unit mass of propellant at a specific temperature.

2. *Covolume (as defined by the Noble-Abel Equation of State)*

The interior ballistician uses the Noble-Abel Equation of State, $P(V-\eta) = n\ R\ T_f$, where η is called the covolume.

3. "Frozen"

The adjective "frozen" refers to the fact that the two heat capacities of the mixture of hot propellant gases are calculated merely as the mole-weighted sum of the heat capacities of the individual components; the chemical equilibria are all considered frozen and make no contribution to the heat capacity.

4. Ratio of "Frozen" Specific Heat Capacities, κ

The ratio of "frozen" specific heats is the ratio between the specific heats of the gas mixture at constant pressure and constant volume in "frozen" chemical composition at the flame temperature.

5. Ratio of Specific Heats at Equilibrium, γ

The ratio of specific heats at equilibrium is defined as the partial derivative of the natural logarithm of pressure with respect to the natural logarithm of density at constant entropy and can be expressed in equation form as

$$\gamma = \left(\frac{\partial \ell n P}{\partial \ell n \rho}\right)_s$$

6. Truncated Virial Equation of State

The equation of state of a gas mixture is assumed to be:

$$\frac{PV}{nRT} = 1 + \frac{nB}{V} + \frac{n^2 C}{V^2}$$

where B and C are called the second and third virial coefficients. The units for B are m^3/mol and for C are (m^6/mol^2).

CALCULATION OF THE RATIO OF "FROZEN" SPECIFIC HEATS

Calculation of κ, the ratio between the specific heats C_p and C_v, is as follows:

The specific heats C_p are used to calculate the respective value for a constant volume in accordance with the relation applying to ideal gases:

$$C_{v\ id} = C_{p\ id} - R$$

The $C_{v\ real}$ holding for real gases can then be calculated from the data of the equation of state for real gases taking into account the dependence on volume and pressure.

$$C_{v\ real} = C_{v\ id} + T\int_{\infty}^{V} \left(\frac{\partial^2 P}{\partial T^2}\right) dV$$

In this case, $\partial^2 P/\partial T^2$ is obtained by double differentiation of the virial equation of state resolved for P.

$$P = nRT\left[\frac{1}{V} + \frac{B(T)}{V^2} + \frac{n^2 C(T)}{V^3}\right]$$

$$\left(\frac{\partial P}{\partial T}\right)_V = \frac{P}{T} + \frac{n^2 RT}{V^2}\left[B'(T) + \frac{nC'(T)}{V}\right]$$

where B' and C' are second and third virial coefficients differentiated with respect to T.

For the second derivative it holds:

$$\frac{\partial^2 P}{\partial T^2} = \frac{2n^2}{V^2}\left[B'(T) + \frac{nC'(T)}{V}\right] + \frac{n^2 RT}{V^2}\left[B''(T) + \frac{nC''(T)}{V}\right]$$

Integration of this partial differential equation finally results in a term which allows $C_{v\ real}$ to be determined:

$$\int_{\infty}^{V} \left(\frac{\partial^2 P}{\partial T^2}\right) dV = -\frac{n^2 R}{V}\left[2B'(T) + TB''(T)\right] + \frac{n^3 R}{2V^2}\left[2C'(T) + TC''(T)\right]$$

Now that $C_{v\ real}$ has become accessible, $C_{p\ real}$ can be found by means of the following relation:

$$C_{p\ real} = C_{v\ real} - T\frac{\left(\frac{\partial P}{\partial T}\right)_V^2}{\left(\frac{\partial P}{\partial V}\right)_T}$$

Again, the two derivatives are accessible through the virial equation of state.

From $C_{p\ real}$ and $C_{v\ real}$ one obtains the ratio of "frozen" specific heat capacities.

$$\kappa_{real} = \frac{C_{p\ real}}{C_{v\ real}}$$

METHOD OF CALCULATION OF SECOND AND THIRD VIRIAL COEFFICIENTS

1. Pure Constituent

This method is due to Hirschfelder (see Bibliography). For non-polar molecules the (6-12) Lennard-Jones potential function is used. This takes into account the mutual attraction between molecules at greater distances and the repulsion associated with close approach. The equation is

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

ϵ is the maximum energy of attraction, or the depth of the potential well, and occurs at $r=2^{1/6}\sigma$. σ is that value of r for which the potential function is zero. The uncertainty in the values of σ and ϵ is approximately 10%.

The second virial coefficient for gases is given by

$$B(T) = 2\pi N \int_{o}^{\infty} [1-e^{-\phi(r)/kT}]\ r^2 dr$$

where k is the Boltzmann constant ($k=1.380658\times10^{-23}$ J/K)

N is the Avogadro constant ($R=kN$) ($N=6.022137\times10^{23}$ mol^{-1})

For non-polar gases this can be expanded to give

$$B(T) = b_o \sum_{j=o}^{\infty} b^{(j)} \left(\frac{kT}{\epsilon}\right)^{-(2j+1)/4}$$

where $b_o = \frac{2}{3}\pi N\sigma^3$

and $b^{(j)} = -\frac{2^{j+1/2}}{4j!}\Gamma\left(\frac{2j-1}{4}\right)$

$b^{(j)}$ is tabulated below

j	$b^{(j)}$	j	$b^{(j)}$	j	$b^{(j)}$	j	$b^{(j)}$
0	1.7330010	11	-6.3872683E-4	21	-9.2768372E-9	31	-1.5742194E-14
1	-2.5636934	12	-2.3818733E-4	22	-2.6673193E-9	32	-3.8108431E-15
2	-8.6650050E-1	13	-8.5982461E-5	23	-7.5168046E-10	33	-9.0935023E-16
3	-4.2728224E-1	14	-3.0100597E-5	24	-2.0778030E-10	34	-2.1397782E-16
4	-2.1662512E-1	15	-1.0236007E-5	25	-5.6376036E-11	35	-4.9670392E-17
5	-1.0682056E-1	16	-3.3872440E-6	26	-1.5024114E-11	36	-1.1378186E-17
6	-5.0545862E-2	17	-1.0913390E-6	27	-3.9350796E-12	37	-2.5730157E-18
7	-2.2890120E-2	18	-3.4305829E-7	28	-1.0135315E-12	38	-5.7457408E-19
8	-9.9286513E-3	19	-1.0530464E-7	29	-2.5684633E-13	39	-1.2674099E-19
9	-4.1329383E-3	20	-3.1597475E-8	30	-6.4073832E-14	40	-2.7623753E-20
10	-1.6547753E-3						

Similarly the third virial coefficient is given by

$$C(T) = b_o^2 \sum_{j=o}^{\infty} c^{(j)} \left(\frac{kT}{\epsilon}\right)^{-(j+1)/2}$$

where $c^{(j)}$ are tabulated below

j	0	1	2	3	4	5	6	7	8
$c^{(j)}$	1.729	-3.203	1.519	0.958	0.429	0.059	-0.140	-0.210	-0.205
j	9	10	11	12	13	14	15	16	17
$c^{(j)}$	-0.168	-0.123	-0.084	-0.059	-0.035	-0.020	-0.011	-0.006	-0.004

For polar molecules the Stockmayer-potential function is used which takes into account dipole-dipole interactions. The function is

$$\phi(r,\theta_1,\theta_2,\phi_2-\phi_1) = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12}-\left(\frac{\sigma}{r}\right)^{6}\right] - \frac{\mu^2}{r^3} g\,(\theta_1,\theta_2,\phi_2-\phi_1)$$

where $g(\theta_1,\theta_2,\phi_2-\phi_1) = 2\cos\theta_1\cos\theta_2-\sin\theta_1\sin\theta_2\cos(\phi_2-\phi_1)$

μ = dipole moment

$\theta_1,\theta_2,\phi_1,\phi_2$ = angles of orientation of the molecules
σ and ϵ have a slightly different interpretation here than in the Lennard-Jones potential.

The equation for B and C are very complicated. The equation for B(T) can be expressed in the form

$$B(T) = b_o B^*(T^*, t^*)$$

where $T^* = Tk/\epsilon$

$$t^* = \sqrt{8}\ \mu^2/(\epsilon\sigma^3)$$

$$\mu^* = \frac{\mu}{\sqrt{\epsilon\sigma^3}}$$

and $C(T) = b_o^2 C^*(T^*, t^*)$

Values of ϵ and σ and μ for some gases are given in Table 1. These are taken from the book by Hirschfelder.

Table 1 Potential Parameters for the Lennard-Jones (6-12) Potential and the Stockmayer Potential

Gas	σ (nm)	ϵ/κ (K)	μ (Debye)
CO_2	0.407	205	-
N_2	0.370	95	-
CO	0.376	100	-
H_2	0.293	37	-
NO	0.317	131	-
O_2	0.358	118	-
CH_4	0.382	148	-
HCl	0.336	328	1.08
NH_3	0.315	358	1.47
H_2O	0.252	775	1.85
CH_3CN	0.402	400	3.5
N_2O	0.385	229	-

Values for other gases can be found from viscosity data and from "Table of Electric Dipole Moments" by L G Webson, MIT, The Technology Press (1948).

B* and C* are tabulated for various values of T* and t* (Tables 2 and 3)

Note that consideration of polarities necessitates using a third parameter, μ (the dipole moment), which is a new source of uncertainty.

In addition Hirschfelder tables give values for C* only over a small range and do not give values for the first and second derivatives of B* and C*.

2. Mixtures

2a. The calculation thus far has been restricted to interactions between molecules of the same chemical species. Empirical combining laws can be used for mixtures. The simplest law was proposed by Corner and is given below

$$nB(T) = \sum_{i=1}^{m} n_i B_i(T)$$

$$nC(T) = \sum_{i=1}^{m} n_i C_i(T)$$

$$n = \sum_{i=1}^{m} n_i$$

2b. This essentially neglects interactions between molecules of different types. A more accurate procedure uses the following

$$n^2B(T) = \sum_{a=1}^{m} \sum_{b=1}^{m} n_a n_b B_{ab}(T)$$

$$n^3C(T) = \sum_{a=1}^{m} \sum_{b=1}^{m} \sum_{c=1}^{m} n_a n_b n_c C_{abc}(T)$$

Here the B_{ab} are determined using the following

$$\sigma_{ab} = (\sigma_a+\sigma_b)/2$$

$$\epsilon_{ab} = (\epsilon_a\epsilon_b)^{1/2}$$

and $t^*_{ab} = \frac{\mu_a \mu_b}{\sqrt{8}\, \epsilon_{ab} \sigma_{ab}^3}$

for interactions between polar-polar and non-polar-non-polar molecules. For interactions between polar(p) and non-polar(n)molecules the following combining laws are used

$$\sigma_{np} = \frac{1}{2} (\sigma_n + \sigma_p) \xi^{-1/6}$$

$$\epsilon_{np} = \sqrt{\epsilon_n \epsilon_p}\, \xi^2$$

where $\xi = [1 + \frac{1}{4} \frac{\alpha_n \mu_p^{*2}}{\sigma_n^3} (\frac{\epsilon_p}{\epsilon_n})^{1/2}]$

where α_n is the polarizability of the non-polar molecule.
The calculation of the $C_{abc}(T)$ is very complicated and it is sufficiently accurate to use the simple combination rule neglecting interactions between molecules of different types.

It can be seen that the consideration of the polarity of certain molecule necessitates taking into account the polarisability of the non-polar molecules, thus giving an additional source of uncertainty Considering all the other sources of uncertainty it is more judicious to consider all the molecules non-polar and to adjust σ and ϵ to minimise the error.

The rigourous calculation method given above increases enormously the complexity for a very small gain in accuracy.

In contrast Corner's method presents a serious disadvantage. The chemical potential of each species can be written as

$$\mu_j = U_j - TS_j + \frac{PV}{n} + RT(\ln (\frac{n_j RT}{PV}) + \frac{n}{V} B_j + \frac{n^2}{2V^2} C_j)$$

The solution procedure of the equation, for the conditions at equilibrium

$$\mu_j + \sum_{i=1}^{l} \lambda_i a_{ij} = 0$$

leads to fairly complicated calculations, especially in the case where the mixture includes condensed species whose molar volume can not be neglected.

2c. Consequently, as in the French code Bagheera and at high pressures above about 400-500MPa, it is preferable to use a different approximation, due to Amagat which is just as simple and better verified than the Corner one. Amagat's approximation leads to much simpler equations than those resulting from Corner's approximation, and is indifferent to the presence of condensed species. Letting

$$V = \sum_{j=1}^{m} n_j V_j$$

$$U = \sum_{j=1}^{m} n_j U_j$$

$$\mu_j = H_j - TS_j + RT \ln \left(\frac{n_j}{n}\right)$$

where V_j is the molar volume.

A first solution consists of using, for the molar volume, a development of virial equation expressed as a function of pressure. It is necessary to use a function complying with the following conditions

$$\left(\frac{\partial V_j}{\partial T}\right)_p > 0 \quad \forall T, \forall P$$

$$\left(\frac{\partial V_j}{\partial p}\right)_T < 0 \quad \forall P, \forall T$$

$$\lim_{p \to \infty} V_j \geq 0 \quad \forall T$$

and, to the 3rd order, must be identical to that of the virial equation of state.

A suitable function is the following

$$V_j = \frac{RT}{P} + \frac{\beta_{1j}}{1+\alpha_{1j}P} - \frac{\beta_{2j}}{1+\alpha_{2j}P}$$

where

$$\beta_{1j} - \beta_{2j} = B_j$$

and

$$\alpha_{1j}\beta_{1j} - \alpha_{2j}\beta_{2j} = \frac{B_j^2 - C_j}{RT}$$

A solution is obtained by dropping the subscript j,

$$\beta_1 = 1.7330010\, b_o \left(\frac{kT}{\epsilon}\right)^{-1/4} \text{ and } \alpha_2 = \beta_2/RT$$

then $\beta_2 = \beta_1 - B$

and $\alpha_1 = \dfrac{\beta^2_2 + B^2 - C}{\beta_1 RT}$

The corrections which need to be made due to the contribution of the term $\beta/(1 + \alpha P)$ are

$$\left(\frac{\partial}{\partial T}\left(\frac{\beta}{1+\alpha P}\right)\right)_p = \frac{\beta'(1+\alpha' P) - \beta\alpha' P}{(1+\alpha P)^2}$$

$$\left(\frac{\partial}{\partial P}\left(\frac{\beta}{1+\alpha P}\right)\right)_T = \frac{-\beta\alpha}{(1+\alpha P)^2}$$

$$U : \frac{\beta(\alpha + T\alpha') - T\beta'\alpha}{\alpha^2} \ln(1+\alpha P) - \frac{\beta(\alpha + T\alpha')P}{\alpha(1+\alpha P)}$$

$$\left(\frac{\partial U}{\partial T}\right)_p : T\,\frac{(\beta\alpha'' - \beta''\alpha)\alpha - 2(\beta\alpha' - \beta'\alpha)\alpha'}{\alpha^3} \ln(1+\alpha P)$$

$$+ \frac{2T(\beta\alpha' - \beta'\alpha)\alpha' - (\beta T\alpha'' + \beta'\alpha)\alpha}{\alpha^2(1+\alpha P)} P + \frac{\beta(\alpha + T\alpha')\alpha' P^2}{\alpha(1+\alpha P)^2}$$

$$\left(\frac{\partial U}{\partial P}\right)_T : -\frac{T\beta'}{1+\alpha P} + \frac{\beta(\alpha + T\alpha')P}{(1+\alpha P)^2}$$

$$\mu_j : \frac{\beta}{\alpha} \ln(1+\alpha P)$$

$$\left(\frac{\partial}{\partial T}\left(\frac{\mu_j}{RT}\right)\right)_p : \frac{T\beta'\alpha - \beta(\alpha + T\alpha')}{RT^2\alpha^2} \ln(1+\alpha P) + \frac{\beta\alpha' P}{RT\alpha(1+\alpha P)}$$

$$\left(\frac{\partial}{\partial P}\left(\frac{\mu_j}{RT}\right)\right)_p : \frac{\beta}{RT(1+\alpha P)}$$

TABLE 1 The Second Virial Coefficient for Polar Gases (The Stockmayer Potential Function)[a]

$B(T) = b_o B^*(T^*;t^*) \qquad T^* = kT/\epsilon$

$= b_o \frac{2}{3}\pi N\sigma^3 \qquad t^* = 8^{-1/2}\mu^{*2} = 8^{-1/2}\mu^2/\epsilon\sigma^3$

$B^*(T^*;t^*)$

T^* \ t^*	0.1	0.2	0.3	0.4	0.5	0.6	0.7
0.30	-31.129	-42.968	-72.01				
0.35	-20.355	-25.879	-38.07	-64.11			
0.40	-14.717	-17.777	-24.090	-36.28	-60.4		
0.45	-11.339	-13.241	-16.985	-23.733	-35.92	-58.8	
0.50	-9.1199	-10.401	-12.841	-17.026	-24.11	-36.36	-59.
0.55	-7.5631	-8.4786	-10.181	-12.996	-17.53	-24.91	-37.3
0.60	-6.4159	-7.1001	-8.3495	-10.360	-13.477	-18.33	-26.0
0.65	-5.5381	-6.0677	-7.0213	-8.5234	-10.789	-14.185	-19.34
0.70	-4.8460	-5.2675	-6.0183	-7.1813	-8.8965	-11.394	-15.05
0.75	-4.2871	-4.6304	-5.2364	-6.1627	-7.5043	-9.413	-12.13
0.80	-3.8268	-4.1116	-4.6110	-5.3659	-6.4433	-7.9476	-10.040
0.85	-3.4414	-3.6815	-4.1000	-4.7271	-5.6113	-6.8267	-8.486
0.90	-3.1142	-3.3193	-3.6758	-4.2045	-4.9432	-5.9457	-7.292
0.95	-2.8330	-3.0103	-3.3166	-3.7695	-4.3961	-5.2373	-6.3523
1.00	-2.5889	-2.7437	-3.0102	-3.4021	-3.9406	-4.6567	-5.5953
1.05	-2.3750	-2.5114	-2.7455	-3.0881	-3.5559	-4.1732	-4.9744
1.10	-2.1862	-2.3072	-2.5145	-2.8167	-3.2271	-3.7649	-4.4572
1.15	-2.0183	-2.1265	-2.3113	-2.5799	-2.9430	-3.4160	-4.0203
1.20	-1.8680	-1.9653	-2.1312	-2.3716	-2.6952	-3.1146	-3.6471
1.25	-1.7328	-1.8208	-1.9706	-2.1870	-2.4773	-2.8519	-3.3249
1.30	-1.6105	-1.6905	-1.8264	-2.0223	-2.2844	-2.6211	-3.0442
1.35	-1.4994	-1.5724	-1.6963	-1.8746	-2.1124	-2.4168	-2.7976
1.40	-1.3980	-1.4649	-1.5784	-1.7413	-1.9581	-2.2348	-2.5795
1.45	-1.3051	-1.3667	-1.4710	-1.6205	-1.8190	-2.0717	-2.3854
1.50	-1.2197	-1.2766	-1.3728	-1.5106	-1.6931	-1.9247	-2.2115
1.55	-1.1410	-1.1937	-1.2827	-1.4101	-1.5785	-1.7917	-2.0549
1.60	-1.0681	-1.1171	-1.1998	-1.3179	-1.4738	-1.6708	-1.9133
1.65	-1.0006	-1.0462	-1.1232	-1.2330	-1.3778	-1.5604	-1.7846
1.70	-0.93775	-0.98038	-1.0523	-1.1547	-1.2896	-1.4594	-1.6674
1.75	-0.87917	-0.91908	-0.98633	-1.0821	-1.2079	-1.3662	-1.5597
1.80	-0.82445	-0.86190	-0.92498	-1.0147	-1.1325	-1.2804	-1.4610
1.85	-0.77322	-0.80844	-0.86772	-0.95197	-1.0625	-1.2011	-1.3699
1.90	-0.72516	-0.75834	-0.81417	-0.89345	-0.99736	-1.1275	-1.2858
1.95	-0.67998	-0.71130	-0.76398	-0.83873	-0.93662	-1.0590	-1.2078
2.00	-0.63745	-0.66707	-0.71686	-0.78747	-0.87985	-0.99526	-1.1353
2.1	-0.55947	-0.58607	-0.63076	-0.69408	-0.77679	-0.87993	-1.0048
2.2	-0.48969	-0.51373	-0.55409	-0.61121	-0.68573	-0.77850	-0.89060

TABLE 1 (Continued)

T* \ t*	0.1	0.2	0.3	0.4	0.5	0.6	0.7
2.3	-0.42693	-0.44877	-0.48540	-0.53721	-0.60472	-0.68865	-0.78989
2.4	-0.37020	-0.39012	-0.42354	-0.47076	-0.53224	-0.60856	-0.70049
2.5	-0.31868	-0.33695	-0.36576	-0.41079	-0.46702	-0.53676	-0.62063
2.6	-0.27172	-0.28852	-0.31668	-0.35642	-0.40807	-0.47205	-0.54292
2.7	-0.22875	-0.24426	-0.27025	-0.30692	-0.35453	-0.41347	-0.48420
2.8	-0.18929	-0.20366	-0.22774	-0.26167	-0.30572	-0.36020	-0.42552
2.9	-0.15295	-0.16630	-0.18867	-0.22018	-0.26106	-0.31159	-0.37210
3.0	-0.11937	-0.13182	-0.15266	-0.18200	-0.22005	-0.26705	-0.32330
3.1	-0.08828	-0.09991	-0.11937	-0.14677	-0.18229	-0.22612	-0.27854
3.2	-0.05941	-0.07030	-0.08852	-0.11417	-0.14740	-0.18839	-0.23738
3.3	-0.03254	-0.04277	-0.05986	-0.08393	-0.11509	-0.15351	-0.19940
3.4	-0.00748	-0.01710	-0.03318	-0.05580	-0.08509	-0.12118	-0.16427
3.5	+0.01594	+0.00688	-0.00828	-0.02959	-0.05717	-0.09115	-0.13169
3.6	0.03787	0.02931	+0.01501	-0.00511	-0.03113	-0.06318	-0.10140
3.7	0.05844	0.05035	0.03682	+0.01780	-0.00680	-0.03708	-0.07318
3.8	0.07778	0.07011	0.05729	0.30928	+0.01598	-0.01268	-0.04684
3.9	0.09597	0.08869	0.07653	0.05944	0.03736	+0.01018	-0.02219
4.0	0.11312	0.10620	0.09465	0.07841	0.05744	0.03163	+0.00091
4.1	0.12930	0.12272	0.11173	0.09628	0.07633	0.05180	0.02259
4.2	0.14460	0.13833	0.12786	0.11314	0.09414	0.07078	0.04298
4.3	0.15907	0.15309	0.14310	0.12907	0.11095	0.08868	0.06218
4.4	0.17279	0.16708	0.15754	0.14414	0.12684	0.10558	0.08029
4.5	0.18580	0.18034	0.17122	0.15841	0.14187	0.12155	0.09740
4.6	0.19815	0.19293	0.18420	0.17194	0.15611	0.13668	0.11357
4.7	0.20990	0.20489	0.19652	0.18478	0.16962	0.15101	0.12888
4.8	0.22107	0.21627	0.20825	0.19699	0.18245	0.16461	0.14340
4.9	0.23172	0.22711	0.21941	0.20860	0.19465	0.17752	0.15718
5.0	0.24187	0.23744	0.23004	0.21965	0.20625	0.18980	0.17026
6.	0.32187	0.31877	0.31360	0.30634	0.29699	0.28552	0.27191
7	0.37532	0.37302	0.36918	0.36380	0.35687	0.34838	0.33832
8	0.41284	0.41106	0.40809	0.40393	0.39857	0.39201	0.38424
9	0.44012	0.43870	0.43633	0.43301	0.42873	0.42349	0.41729
10	0.46049	0.45932	0.45738	0.45466	0.45116	0.44687	0.44179
20	0.52527	0.52495	0.52441	0.52367	0.52271	0.52153	0.52014
30	0.52687	0.52672	0.52647	0.52611	0.52566	0.52510	0.52444
40	0.51854	0.51845	0.51830	0.51809	0.51782	0.51749	0.51710
50	0.50834	0.50828	0.50818	0.50804	0.50876	0.50764	0.50738
60	0.49820	0.49815	0.49808	0.49798	0.49785	0.49769	0.49750
70	0.48864	0.48861	0.48855	0.48847	0.48838	0.48826	0.48811
80	0.47978	0.47976	0.47971	0.47965	0.47957	0.47948	0.47937
90	0.47161	0.47159	0.47155	0.47150	0.47144	0.47136	0.47127
100	0.46406	0.46405	0.46402	0.46398	0.46392	0.46386	0.46379
200	0.41143	0.41142	0.41142	0.41140	0.41139	0.41137	0.41135
300	0.38013	0.38012	0.38012	0.38011	0.38011	0.38010	0.38009
400	0.35835	0.35835	0.35835	0.35834	0.35834	0.35833	0.35833

TABLE 1 (Continued)

T* \ t*	0.8	0.9	1.0	1.1	1.2	1.3	1.4	1.5
0.55	-58.8							
0.60	-38.5	-59.7						
0.65	-27.3	-40.0						
0.70	-20.50	-28.8	-41.8					
0.75	-16.05	-21.78	-30.4	-43.5				
0.80	-12.973	-17.14	-23.2	-32.0	-45.8			
0.85	-10.759	-13.90	-18.4	-24.7	-34.4	-47.0		
0.90	-9.103	-11.612	-14.92	-19.61	-26.3	-35.7	50.3	
0.95	-7.828	-9.790	-12.42	-16.00	-21.0	-27.9	37.8	-52.0
1.00	-6.820	-8.440	-10.54	-13.36	-17.2	-22.3	-29.8	-40.0
1.05	-6.008	-7.342	-9.08	-11.35	-14.3	-18.4	-24.3	-31.0
1.10	-5.3413	-6.4696	-7.915	-9.780	-12.21	-15.42	-19.6	-25.4
1.15	-4.7855	-5.7520	-6.976	-8.534	-10.53	-13.13	-16.5	-21.1
1.20	-4.3161	-5.1537	-6.203	-7.524	-9.20	-11.34	-14.1	-17.7
1.25	-3.9152	-4.6483	-5.559	-6.693	-8.11	-9.90	-12.2	-15.1
1.30	-3.5690	-4.2164	-5.014	-5.998	-7.21	-8.74	-10.7	-13.1
1.35	-3.2676	-3.8438	-4.5484	-5.4111	-6.471	-7.780	-9.41	-11.46
1.40	-3.0030	-3.5193	-4.1466	-4.9092	-5.839	-6.976	-8.38	-10.12
1.45	-2.7691	-3.2345	-3.7970	-4.4762	-5.298	-6.296	-7.51	-9.00
1.50	-2.5609	-2.9829	-3.4903	-4.0994	-4.831	-5.714	-6.78	-8.08
1.55	-2.3745	-2.7591	-3.2192	-3.7688	-4.426	-5.212	-6.15	-7.29
1.60	-2.2069	-2.5589	-2.9783	-3.4768	-4.069	-4.774	-5.612	-6.62
1.65	-2.0554	-2.3788	-2.7629	-3.2173	-3.7548	-4.3909	-5.145	-6.045
1.70	-1.9180	-2.2165	-2.5697	-2.9860	-3.4760	-4.0532	-4.735	-5.541
1.75	-1.7923	-2.0685	-2.3943	-2.7770	-3.2256	-3.7517	-4.370	-5.097
1.80	-1.6775	-1.9340	-2.2357	-2.5889	-3.0014	-3.4831	-4.046	-4.706
1.85	-1.5720	-1.8110	-2.0912	-2.4183	-2.7990	-3.2419	-3.758	-4.359
1.90	-1.4749	-1.6981	-1.9591	-2.2630	-2.6156	-3.0244	-3.498	-4.049
1.95	-1.3852	-1.5941	-1.8380	-2.1211	-2.4487	-2.8273	-3.265	-3.771
2.00	-1.3021	-1.4982	-1.7265	-1.9910	-2.2963	-2.6479	-3.053	-3.520
2.1	-1.1531	-1.3268	-1.5285	-1.7610	-2.0282	-2.3342	-2.6846	-3.0857
2.2	-1.0234	-1.1785	-1.3580	-1.5643	-1.8002	-2.0693	-2.3758	-2.7248
2.3	-0.90957	-1.0490	-1.2100	-1.3943	-1.6044	-1.8431	-2.1138	-2.4204
2.4	-0.80895	-0.93509	-1.0803	-1.2461	-1.4345	-1.6479	-1.8889	-2.1606
2.5	-0.71944	-0.83413	-0.96584	-1.1159	-1.2860	-1.4780	-1.6940	-1.9368
2.6	-0.63934	-0.74412	-0.86421	-1.0008	-1.1551	-1.3289	-1.5239	-1.7423
2.7	-0.56729	-0.66342	-0.77343	-0.89828	-1.0391	-1.1972	-1.3742	-1.5719
2.8	-0.50216	-0.59072	-0.69191	-0.80654	-0.93559	-1.0802	-1.2416	-1.4215
2.9	-0.44304	-0.52492	-0.61833	-0.72400	-0.84275	-0.97554	-1.1235	-1.2879
3.0	-0.38917	-0.46511	-0.55165	-0.64940	-0.75908	-0.88152	-1.0177	-1.1687
3.1	-0.33989	-0.41054	-0.49096	-0.58168	-0.68333	-0.79663	-0.92240	-1.0616
3.2	-0.29466	-0.36057	-0.43552	-0.51998	-0.61449	-0.71967	-0.83625	-0.96505
3.3	-0.25302	-0.31468	-0.38472	-0.46355	-0.55167	-0.64962	-0.75801	-0.87758
3.4	-0.21459	-0.27239	-0.33800	-0.41179	-0.49417	-0.58562	-0.68671	-0.79805
3.5	-0.17900	-0.23332	-0.29493	-0.36415	-0.44135	-0.52697	-0.62149	-0.72546
3.6	-0.14598	-0.19713	-0.25510	-0.32018	-0.39270	-0.47305	-0.56164	-0.65899

TABLE 1 (Continued)

T* \ t*	0.8	0.9	1.0	1.1	1.2	1.3	1.4	1.5
3.7	-0.11527	-0.16352	-0.21818	-0.27949	-0.34776	-0.42333	-0.50657	-0.59792
3.8	-0.08664	-0.13225	-0.18388	-0.24176	-0.30615	-0.37736	-0.45574	-0.54166
3.9	-0.05989	-0.10308	-0.15193	-0.20667	-0.26752	-0.33476	-0.40870	-0.48968
4.0	-0.03486	-0.07582	-0.12213	-0.17397	-0.23158	-0.29519	-0.36507	-0.44155
4.1	-0.01140	-0.05030	-0.09426	-0.14345	-0.19807	-0.25834	-0.32451	-0.39687
4.2	+0.01064	-0.02636	-0.06815	-0.11490	-0.16677	-0.22397	-0.28673	-0.35530
4.3	0.03137	-0.00387	-0.04366	-0.08814	-0.13747	-0.19184	-0.25145	-0.31654
4.4	0.05089	+0.01729	-0.02064	-0.06302	-0.11000	-0.16175	-0.21846	-0.28033
4.5	0.06932	0.03723	+0.00103	-0.03941	-0.08421	-0.13353	-0.18755	-0.24645
4.6	0.08672	0.05605	0.02145	-0.01717	-0.05995	-0.10702	-0.15854	-0.21469
4.7	0.10318	0.07383	0.04073	+0.00380	-0.03709	-0.08207	-0.13127	-0.18486
4.8	0.11877	0.09065	0.05896	0.02360	-0.01554	-0.05856	-0.10560	-0.15681
4.9	0.13355	0.10659	0.07620	0.04232	+0.00483	-0.03637	-0.08140	-0.13039
5.0	0.14758	0.12170	0.09255	0.06004	0.02409	-0.01540	-0.05855	-0.10548
6	0.25614	0.23818	0.21799	0.19554	0.17077	+0.14364	+0.11409	+0.08206
7	0.32667	0.31341	0.29853	0.28199	0.26379	0.24389	0.22225	0.19885
8	0.37524	0.36502	0.35355	0.34082	0.32682	0.31154	0.29494	0.27702
9	0.41012	0.40197	0.39283	0.38270	0.37157	0.35942	0.34625	0.33203
10	0.43593	0.42927	0.42180	0.41353	0.40444	0.39453	0.38379	0.37221
20	0.51854	0.51672	0.51468	0.51243	0.50996	0.50728	0.50438	0.50125
30	0.52367	0.52281	0.52184	0.52077	0.51960	0.51833	0.51695	0.51547
40	0.51665	0.51613	0.51556	0.51493	0.51423	0.51348	0.51266	0.51179
50	0.50707	0.50673	0.50635	0.50593	0.50546	0.50496	0.50441	0.50383
60	0.49729	0.49704	0.49676	0.49646	0.49613	0.49576	0.49537	0.49495
70	0.48795	0.48776	0.48755	0.48732	0.48707	0.48679	0.48650	0.48618
80	0.47924	0.47909	0.47893	0.47874	0.47854	0.47833	0.47810	0.47784
90	0.47117	0.47105	0.47091	0.47077	0.47061	0.47043	0.47024	0.47004
100	0.46370	0.46360	0.46349	0.46337	0.46323	0.46309	0.46293	0.46276
200	0.41132	0.41129	0.41126	0.41123	0.41119	0.41115	0.41110	0.41105
300	0.38008	0.38006	0.38005	0.38003	0.38001	0.37999	0.37997	0.37994
400	0.35832	0.35831	0.35830	0.35829	0.35828	0.35827	0.35825	0.35824

TABLE 2 The Third Virial Coefficient for Polar Gases (The Stockmayer Potential Function)

$C(T) = b_o^2 C^*(T^*;t^*)$ $\quad T^* = kT/\epsilon$ $\quad b_o = \frac{2}{3}\pi N\sigma^3$ $\quad t^* = 8^{-1/2}\,\mu^2/\epsilon\sigma^3$

$C^*(T^*;t^*)$

T^* \ t^*	0.0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	1.0	1.2
1.0	0.4297	0.4440	0.5304	0.740							
1.2	0.5924	0.6177	0.7162	0.9216	1.268	1.78	2.5	3.4	4.6	7.	
1.4	0.5683	0.5900	0.6679	0.8221	1.075	1.451	2.0	2.7	3.7	6.3	9.
1.6	0.5180	0.5351	0.5940	0.7075	0.8899	1.158	1.53	2.03	2.69	4.72	7.0
1.8	0.4728	0.4861	0.5311	0.6161	0.7507	0.9455	1.214	1.572	2.03	3.36	5.2
2.0	0.4371	0.4476	0.4826	0.5478	0.6496	0.7957	0.995	1.257	1.595	2.46	4.0
2.5	0.3811	0.3873	0.4076	0.4445	0.5195	0.5807	0.6871	0.825	0.999	1.482	2.19
3.0	0.3523	0.3563	0.3692	0.3924	0.4275	0.4761	0.5403	0.6223	0.7248	1.002	1.401
4.0	0.3266	0.3286	0.3350	0.3463	0.3630	0.3859	0.4156	0.4529	0.4986	0.6194	0.7857
6.0	0.3077	0.3085	0.3109	0.3151	0.3213	0.3296	0.3401	0.3532	0.3690	0.4095	0.4640
8.0	0.2962	0.2966	0.2978	0.3000	0.3031	0.3072	0.3124	0.3188	0.3265	0.3459	0.3715
10.0	0.2861	0.2863	0.2871	0.2884	0.2902	0.2926	0.2957	0.2995	0.3039	0.3151	0.3297

COEFFICIENTS OF HEAT CAPACITY, ENTHALPY AND ENTROPY

The primary reference source for this data is the JANAF tables. The secondary reference is the Nasa-Lewis expansion coefficients which are based on the JANAF tables.

KEY

LINE 1: In order: Name, Source, Coded formula, Phase, Temp range, and Formula Wt.

SOURCES:
- J = JANAF
- L = unpublished data calculated at LEWIS RESEARCH CENTER
- RUS = Russian literature

The number refers to the month and year the data were published or calculated (12/65 is December 1965).

PHASE:
- G = gas
- S = solid
- L = liquid

EXAMPLE

NAME	SOURCE	CODED FORMULA	P	TEMP. RANGE	FORM. WT
FORMALDEHYDE	J 3/61	C 1.H 2.0 1.Ø Ø.	G	3ØØ.ØØØ 5ØØØ.ØØØ	3Ø.Ø262Ø

LINES 2-4: The 7 coefficients for T => 1ØØØK, followed by the 7 coefficients for T <= 1ØØØ K

```
FORMALDEHYDE      J 3/61C  1.H  2.0  1.Ø  Ø.G   3ØØ.ØØØ  5ØØØ.ØØØ    3Ø.Ø262Ø  1
 Ø.28364249E Ø1 Ø.686Ø5298E-Ø2-Ø.26882647E-Ø5 Ø.47971258E-Ø9-Ø.32118406E-13    2
-Ø.15236Ø31E Ø5 Ø.78531169E Ø1 Ø.37963783E Ø1-Ø.257Ø1785E-Ø2 Ø.18548815E-Ø4    3
-Ø.17869177E-Ø7 Ø.55Ø4451E-11-Ø.15Ø88947E Ø5 Ø.47548163E Ø1     Ø.ØØØØØØØØ    4

FORMIC ACID       L 4/85C  1.H  2.0  2.   Ø.G   3ØØ.ØØØ  5ØØØ.ØØØ    46.Ø256Ø  1
 Ø.57752972E Ø1 Ø.75786225E-Ø2-Ø.3115144ØE-Ø5 Ø.54887672E-Ø9-Ø.35Ø43661E-13    2
-Ø.48186Ø55E Ø5-Ø.646Ø9318E Ø1 Ø.214Ø2845E Ø1 Ø.11Ø24252E-Ø1 Ø.2993Ø725E-Ø5    3
-Ø.8553652ØE-Ø8 Ø.31486766E-11-Ø.46671Ø35E Ø5 Ø.14387356E Ø2-Ø.45531584E Ø5    4

CH4               L 5/84C  1.H  4.   Ø.   Ø.G   3ØØ.ØØØ  5ØØØ.ØØØ    16.Ø426Ø  1
 Ø.21737833E Ø1 Ø.89936592E-Ø2-Ø.27855467E-Ø5 Ø.39775117E-Ø9-Ø.19976425E-13    2
-Ø.1Ø216566E Ø5 Ø.7Ø773563E Ø1 Ø.2Ø428148E Ø1 Ø.25153728E-Ø2 Ø.79Ø85839E-Ø5    3
-Ø.47495483E-Ø8 Ø.1424491ØE-12-Ø.1ØØ56824E Ø5 Ø.45714579E Ø1-Ø.9ØØ51691E Ø4    4
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METHANOL          L 9/85C  1.H  4.0  1.   Ø.G   3ØØ.ØØØ  5ØØØ.ØØØ    32.Ø42ØØ  1
 Ø.4Ø351191E Ø1 Ø.93647Ø4E-Ø2-Ø.3Ø427ØØØE-Ø5 Ø.43397752E-Ø9-Ø.22Ø82799E-13    2
-Ø.2616Ø1Ø9E Ø5 Ø.23459Ø85E Ø1 Ø.26642971E Ø1 Ø.73133595E-Ø2 Ø.72366365E-Ø5    3
-Ø.8859562ØE-Ø8 Ø.24143231E-11-Ø.25353945E Ø5 Ø.11214846E Ø2-Ø.24184888E Ø5    4

CO                J 9/65C  1.O  1.   Ø.   Ø.G   3ØØ.ØØØ  5ØØØ.ØØØ    28.Ø1Ø4Ø  1
 Ø.29840696E Ø1 Ø.1489139ØE-Ø2-Ø.57899684E-Ø6 Ø.1Ø364577E-Ø9-Ø.6935355ØE-14    2
-Ø.14245228E Ø5 Ø.63479156E Ø1 Ø.371ØØ928E Ø1-Ø.16199Ø64E-Ø2 Ø.36923594E-Ø5    3
-Ø.2Ø319674E-Ø8 Ø.23953344E-12-Ø.14356310E Ø5 Ø.29555351E Ø1     Ø.ØØØØØØØØ    4

COS               J 3/61C  1.O  1.S  1.   Ø.G   3ØØ.ØØØ  5ØØØ.ØØØ    6Ø.Ø7Ø4Ø  1
 Ø.52392ØØØE Ø1 Ø.241ØØ584E-Ø2-Ø.96Ø64522E-Ø6 Ø.17778347E-Ø9-Ø.12235Ø4E-13    2
-Ø.18480455E Ø5-Ø.3Ø91Ø517E Ø1 Ø.24625321E Ø1 Ø.11947992E-Ø1-Ø.1379437ØE-Ø4    3
 Ø.8Ø7Ø7736E-Ø8-Ø.18327653E-11-Ø.17Ø3987E Ø5 Ø.1Ø792556E Ø2     Ø.ØØØØØØØØ    4

CO2               J 9/65C  1.O  2.   Ø.   Ø.G   3ØØ.ØØØ  5ØØØ.ØØØ    44.ØØ98Ø  1
 Ø.4460Ø841E Ø1 Ø.3Ø981719E-Ø2-Ø.12392571E-Ø5 Ø.22741325E-Ø9-Ø.15525954E-13    2
-Ø.48961442E Ø5-Ø.98635982E ØØ Ø.24ØØ7797E Ø1 Ø.87350957E-Ø2-Ø.66Ø7Ø878E-Ø5    3
 Ø.2ØØ21861E-Ø8 Ø.63274Ø39E-15-Ø.48377527E Ø5 Ø.96951457E Ø1-Ø.94Ø54ØØØE Ø5    4

H                 J 3/77H  1.   Ø.   Ø.   Ø.G   3ØØ.ØØØ  5ØØØ.ØØØ     1.ØØ79Ø  1
 Ø.25ØØØØØØE Ø1     Ø.ØØØØØØØØ     Ø.ØØØØØØØØ     Ø.ØØØØØØØØ     Ø.ØØØØØØØØ    2
 Ø.2547439ØE Ø5-Ø.45989841E ØØ Ø.25ØØØØØØE Ø1     Ø.ØØØØØØØØ     Ø.ØØØØØØØØ    3
 Ø.ØØØØØØØØ     Ø.ØØØØØØØØ     Ø.25474390E Ø5-Ø.45989841E ØØ     Ø.ØØØØØØØØ    4

HCN               L12/69H  1.C  1.N  1.Ø  Ø.G   3ØØ.ØØØ  5ØØØ.ØØØ    27.Ø256Ø  1
 Ø.37Ø68121E Ø1 Ø.33382Ø3E-Ø2-Ø.11913320E-Ø5 Ø.19992917E-Ø9-Ø.12826452E-13    2
 Ø.14962636E Ø5 Ø.2Ø794Ø4E Ø1 Ø.24513556E Ø1 Ø.87Ø8371E-Ø2-Ø.1ØØ94Ø3E-Ø4    3
 Ø.67255698E-Ø8-Ø.17626959E-11 Ø.15213ØØ2E Ø5 Ø.8Ø83Ø085E Ø1     Ø.ØØØØØØØØ    4

HCO RAD           J12/7ØH  1.C  1.O  1.Ø  Ø.G   3ØØ.ØØØ  5ØØØ.ØØØ    29.Ø183Ø  1
 Ø.34738348E Ø1 Ø.34370227E-Ø2-Ø.13632664E-Ø5 Ø.24928645E-Ø9-Ø.17044331E-13    2
 Ø.39594ØØ5E Ø4 Ø.6Ø453340E Ø1 Ø.3884Ø192E Ø1-Ø.82974448E-Ø3 Ø.779ØØ8Ø9E-Ø5    3
-Ø.7Ø616962E-Ø8 Ø.19971730E-11 Ø.4Ø5638Ø0E Ø4 Ø.48354133E Ø1     Ø.ØØØØØØØØ    4

HNCO              J12/7ØH  1.N  1.C  1.O  1.G   3ØØ.ØØØ  5ØØØ.ØØØ    43.Ø25ØØ  1
 Ø.513ØØ39ØE Ø1 Ø.43551371E-Ø2-Ø.16269Ø22E-Ø5 Ø.28Ø3569ØE-Ø9-Ø.18276Ø37E-13    2
-Ø.141Ø1787E Ø5-Ø.22Ø1Ø995E Ø1 Ø.23722164E Ø1 Ø.13664Ø4ØE-Ø1-Ø.13323158E-Ø4    3
 Ø.64475457E-Ø8-Ø.1Ø4Ø2894E-11-Ø.13437Ø59E Ø5 Ø.11588263E Ø2     Ø.ØØØØØØØØ    4
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HNO               RUS 78H  1.N  1.O  1.   Ø.G   298.15Ø  5ØØØ.ØØØ    31.Ø14ØØ  1
 Ø.33290296E Ø1 Ø.27934155E-Ø2-Ø.32555667E-Ø6-Ø.61905698E-1Ø Ø.1Ø4Ø3731E-13    2
 Ø.11117372E Ø5 Ø.66846734E Ø1 Ø.4597945ØE Ø1-Ø.61655ØØE-Ø2 Ø.19782938E-Ø4    3
-Ø.18561387E-Ø7 Ø.6Ø914812E-11 Ø.11Ø33783E Ø5 Ø.14Ø2991E Ø1 Ø.12271ØØE Ø5    4

HNO2              RUS 78H  1.N  1.O  2.   Ø.G   298.15Ø  5ØØØ.ØØØ    47.Ø134Ø  1
 Ø.55Ø79788E Ø1 Ø.42Ø14ØØ7E-Ø2-Ø.16471376E-Ø5 Ø.2977413ØE-Ø9-Ø.2Ø3Ø8472E-13    2
-Ø.11459164E Ø5-Ø.25Ø59193E Ø1 Ø.25418194E Ø1 Ø.1318547ØE-Ø1-Ø.1154Ø6Ø6E-Ø4    3
 Ø.47Ø3251ØE-Ø8-Ø.58616939E-12-Ø.1Ø687376E Ø5 Ø.126Ø13Ø1E Ø2-Ø.94360387E Ø4    4

H2                J 3/77H  2.   Ø.   Ø.   Ø.G   3ØØ.ØØØ  5ØØØ.ØØØ     2.Ø158Ø  1
 Ø.3Ø558196E Ø1 Ø.5974Ø4ØØE-Ø3-Ø.16747471E-Ø8-Ø.21247544E-1Ø Ø.25195487E-14    2
-Ø.86168476E Ø3-Ø.172Ø7Ø73E Ø1 Ø.29432327E Ø1 Ø.34815Ø9E-Ø2-Ø.77713819E-Ø5    3
 Ø.74997496E-Ø8-Ø.252Ø3379E-11-Ø.97695413E Ø3-Ø.18186137E Ø1     Ø.ØØØØØØØØ    4

H2O               J 3/79H  2.O  1.   Ø.   Ø.G   3ØØ.ØØØ  5ØØØ.ØØØ    18.Ø152Ø  1
 Ø.26340654E Ø1 Ø.31121899E-Ø2-Ø.9Ø278449E-Ø6 Ø.12673Ø54E-Ø9-Ø.69164732E-14    2
-Ø.29876258E Ø5 Ø.7Ø823873E Ø1 Ø.41675564E Ø1-Ø.181Ø6868E-Ø2 Ø.5945Ø878E-Ø5    3
-Ø.48670871E-Ø8 Ø.15284144E-11-Ø.3Ø289546E Ø5-Ø.73Ø87997E ØØ     Ø.ØØØØØØØØ    4


H2S               J 6/77H  2.S  1.   Ø.   Ø.G   3ØØ.ØØØ  5ØØØ.ØØØ    34.Ø758Ø  1
 Ø.27452199E Ø1 Ø.4Ø434607E-Ø2-Ø.15384510E-Ø5 Ø.2752Ø249E-Ø9-Ø.18592Ø95E-13    2
-Ø.34199444E Ø4 Ø.8Ø412439E Ø1 Ø.39323476E Ø1-Ø.5Ø26Ø9Ø5E-Ø3 Ø.45928473E-Ø5    3
-Ø.318Ø7214E-Ø8 Ø.66497561E-12-Ø.365Ø5359E Ø4 Ø.23Ø23599E Ø1     Ø.ØØØØØØØØ    4

K                 J 6/62K  1.   Ø.   Ø.   Ø.G   3ØØ.ØØØ  5ØØØ.ØØØ    39.Ø983Ø  1
 Ø.2567365ØE Ø1-Ø.14933596E-Ø3 Ø.12342444E-Ø6-Ø.5339424ØE-1Ø Ø.11948426E-13    2
 Ø.9955Ø531E Ø4 Ø.46642Ø81E Ø1 Ø.24930967E Ø1 Ø.5Ø164177E-Ø4-Ø.12751224E-Ø6    3
 Ø.13540491E-Ø9-Ø.51145936E-13 Ø.99786360E Ø4 Ø.5Ø560438E Ø1     Ø.ØØØØØØØØ    4

KCN               J 3/66K  1.C  1.N  1.   Ø.G   3ØØ.ØØØ  5ØØØ.ØØØ    65.116ØØ  1
 Ø.58ØØ712ØE Ø1 Ø.172ØØ786E-Ø2-Ø.7Ø791Ø74E-Ø6 Ø.13199247E-Ø9-Ø.919Ø8323E-14    2
 Ø.77272628E Ø4-Ø.31719981E Ø1 Ø.5Ø81Ø711E Ø1 Ø.55265956E-Ø2-Ø.91157121E-Ø5    3
 Ø.84488817E-Ø8-Ø.3ØØ51548E-11 Ø.78662161E Ø4 Ø.17318296E ØØ     Ø.ØØØØØØØØ    4

KH                J 3/63K  1.H  1.   Ø.   Ø.G   3ØØ.ØØØ  5ØØØ.ØØØ    40.1Ø62Ø  1
 Ø.396Ø3386E Ø1 Ø.72190323E-Ø3-Ø.26918715E-Ø6 Ø.526173ØØE-1Ø-Ø.37872683E-14    2
 Ø.135Ø1837E Ø5 Ø.8421Ø86ØE ØØ Ø.28157756E Ø1 Ø.3987106ØE-Ø2-Ø.3341Ø548E-Ø5    3
 Ø.886Ø2942E-Ø9 Ø.114Ø2847E-12 Ø.138Ø5838E Ø5 Ø.6712Ø145E Ø1     Ø.ØØØØØØØØ    4
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KOH                 J12/70K  1.0  1.H  1.Ø  Ø.G   3ØØ.ØØØ  5ØØØ.ØØØ    56.1Ø56Ø  1
 Ø.564ØØ949E Ø1 Ø.12510226E-Ø2-Ø.34984547E-Ø6 Ø.44566993E-1Ø-Ø.2Ø87Ø279E-14    2
-Ø.29698732E Ø5 Ø.4Ø568187E Ø1 Ø.4Ø733441E Ø1 Ø.97217945E-Ø2-Ø.15988Ø4E-Ø4    3
 Ø.12148353E-Ø7-Ø.337Ø9342E-11-Ø.295Ø6558E Ø5 Ø.29222373E Ø1     Ø.ØØØØØØØØ    4

NH2                 RUS 78N  1.H  2.   Ø.   Ø.G   298.15Ø  5ØØØ.ØØØ    16.Ø225Ø  1
 Ø.26364Ø64E Ø1 Ø.36Ø1Ø668E-Ø2-Ø.119Ø3551E-Ø5 Ø.2Ø318811E-Ø9-Ø.13761458E-13    2
 Ø.21997335E Ø5 Ø.75913284E Ø1 Ø.41350202E Ø1-Ø.15922608E-Ø2 Ø.57789ØØE-Ø5    3
-Ø.41822865E-Ø8 Ø.1Ø971418E-11 Ø.21646478E Ø5 Ø.132Ø55Ø5E ØØ Ø.22851898E Ø5    4

NH3                 J 6/77N  1.H  3.   Ø.   Ø.G   298.15Ø  5ØØØ.ØØØ    17.Ø3Ø4Ø  1
 Ø.23172706E Ø1 Ø.62831974E-Ø2-Ø.21245407E-Ø5 Ø.34ØØ4532E-Ø9-Ø.21457956E-13    2
-Ø.64266256E Ø4 Ø.82962119E Ø1 Ø.37912795E Ø1-Ø.94953142E-Ø3 Ø.12Ø79642E-Ø4    3
-Ø.12401333E-Ø7 Ø.42744577E-11-Ø.66928361E Ø4 Ø.14179Ø45E Ø1-Ø.552Ø3546E Ø4    4

NO                  RUS 78N  1.O  1.   Ø.   Ø.G   298.15Ø  5ØØØ.ØØØ    3Ø.ØØ61Ø  1
 Ø.31486543E Ø1 Ø.14151823E-Ø2-Ø.57574881E-Ø6 Ø.1Ø738529E-Ø9-Ø.739ØØ199E-14    2
 Ø.99610628E Ø4 Ø.69670936E Ø1 Ø.42484931E Ø1-Ø.48661106E-Ø2 Ø.11634155E-Ø4    3
-Ø.99768494E-Ø8 Ø.3Ø483948E-11 Ø.98418Ø42E Ø4 Ø.21434823E Ø1 Ø.1Ø976729E Ø5    4

N2                  J 3/77N  2.   Ø.   Ø.   Ø.G   298.15Ø  5ØØØ.ØØØ    28.Ø134Ø  1
 Ø.28536374E Ø1 Ø.16Ø14368E-Ø2-Ø.62888336E-Ø6 Ø.11428932E-Ø9-Ø.77953822E-14    2
-Ø.89Ø2Ø951E Ø3 Ø.63942727E Ø1 Ø.37Ø34288E Ø1-Ø.14179405E-Ø2 Ø.28625Ø94E-Ø5    3
-Ø.12Ø18374E-Ø8-Ø.13475522E-13-Ø.1Ø639421E Ø4 Ø.22379315E Ø1     Ø.ØØØØØØØØ    4

O                   J 3/77O  1.   Ø.   Ø.   Ø.G   3ØØ.ØØØ  5ØØØ.ØØØ    15.9994Ø  1
 Ø.25342961E Ø1-Ø.1247817ØE-Ø4-Ø.12562724E-Ø7 Ø.69Ø29862E-11-Ø.63797Ø95E-15    2
 Ø.29231108E Ø5 Ø.49628591E Ø1 Ø.3Ø3Ø94Ø1E Ø1-Ø.22525853E-Ø2 Ø.3982454ØE-Ø5    3
-Ø.326Ø4921E-Ø8 Ø.1Ø152Ø35E-11 Ø.29136526E Ø5 Ø.26Ø99342E Ø1     Ø.ØØØØØØØØ    4

OH                  J 6/77O  1.H  1.   Ø.   Ø.G   3ØØ.ØØØ  5ØØØ.ØØØ    17.ØØ73Ø  1
 Ø.28897814E Ø1 Ø.1ØØØ5879E-Ø2-Ø.22Ø48807E-Ø6 Ø.2Ø191288E-1Ø-Ø.394Ø9831E-15    2
 Ø.38857Ø42E Ø4 Ø.55566427E Ø1 Ø.38737300E Ø1-Ø.13393772E-Ø2 Ø.16348351E-Ø5    3
-Ø.52133639E-Ø9 Ø.41826974E-13 Ø.35802348E Ø4 Ø.342Ø2406E ØØ     Ø.ØØØØØØØØ

O2                  J 3/77O  2.   Ø.   Ø.   Ø.G   3ØØ.ØØØ  5ØØØ.ØØØ    31.9988Ø  1
 Ø.36122139E Ø1 Ø.74853166E-Ø3-Ø.19820647E-Ø6 Ø.33749008E-1Ø-Ø.2390737ØE-14    2
-Ø.11978151E Ø4 Ø.367Ø3307E Ø1 Ø.37837135E Ø1-Ø.3Ø233634E-Ø2 Ø.99492751E-Ø5    3
-Ø.98189101E-Ø8 Ø.33Ø31825E-11-Ø.1Ø638107E Ø4 Ø.36416345E Ø1     Ø.ØØØØØØØØ    4
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S                J 9/77S  1.   Ø.   Ø.   Ø.G   3ØØ.ØØØ  5ØØØ.ØØØ    32.Ø6ØØØ  1
 Ø.29171783E Ø1-Ø.57194760E-Ø3 Ø.28890940E-Ø6-Ø.52911339E-1Ø Ø.33647474E-14    2
 Ø.32484363E Ø5 Ø.37503810E Ø1 Ø.28695579E Ø1 Ø.63609306E-Ø3-Ø.34420074E-Ø5    3
 Ø.40332507E-Ø8-Ø.15123007E-11 Ø.32453195E Ø5 Ø.37536114E Ø1     Ø.ØØØØØØØØ    4

SH               J 6/77S  1.H  1.   Ø.   Ø.G   3ØØ.ØØØ  5ØØØ.ØØØ    33.Ø679Ø  1
 Ø.3ØØ14537E Ø1 Ø.13394957E-Ø2-Ø.46789663E-Ø6 Ø.7880401Ø5E-1Ø-Ø.5Ø28Ø453E-14    2
 Ø.159Ø532ØE Ø5 Ø.62711902E Ø1 Ø.44420322E Ø1-Ø.24359197E-Ø2 Ø.19Ø64576E-Ø5    3
 Ø.99166630E-Ø9-Ø.95740762E-12 Ø.15523258E Ø5-Ø.11579273E Ø1     Ø.ØØØØØØØØ    4

SO2              J 6/61S  1.O  2.   Ø.   Ø.G   3ØØ.ØØØ  5ØØØ.ØØØ    64.Ø588Ø  1
 Ø.52451364E Ø1 Ø.19704204E-Ø2-Ø.8Ø375769E-Ø6 Ø.15149969E-Ø9-Ø.1Ø558ØØ4E-13    2
-Ø.37558227E Ø5-Ø.10873524E Ø1 Ø.32665338E Ø1 Ø.53237902E-Ø2 Ø.68437552E-Ø6    3
-Ø.52810047E-Ø8 Ø.25590454E-11-Ø.36908148E Ø5 Ø.96513476E Ø1     Ø.ØØØØØØØØ    4

S2               J 9/77S  2.   Ø.   Ø.   Ø.G   3ØØ.ØØØ  5ØØØ.ØØØ    64.12ØØØ  1
 Ø.39886Ø69E Ø1 Ø.55775Ø51E-Ø3-Ø.5Ø189278E-Ø7-Ø.1547Ø319E-1Ø Ø.26661771E-14    2
 Ø.14198Ø15E Ø5 Ø.44777479E Ø1 Ø.28585754E Ø1 Ø.51758355E-Ø2-Ø.65493434E-Ø5    3
 Ø.33998643E-Ø8-Ø.4Ø156766E-12 Ø.14412402E Ø5 Ø.98778348E Ø1     Ø.ØØØØØØØØ    4

S2O              J 9/65S  2.O  1.   Ø.   Ø.G   3ØØ.ØØØ  5ØØØ.ØØØ    8Ø.1194Ø  1
 Ø.59Ø37524E Ø1 Ø.12369975E-Ø2-Ø.5457Ø79ØE-Ø6 Ø.1Ø659842E-Ø9-Ø.76688243E-14    2
-Ø.87752Ø9ØE Ø4-Ø.22833860E Ø1 Ø.28414257E Ø1 Ø.12188410E-Ø1-Ø.16ØØØ241E-Ø4    3
 Ø.1Ø3Ø9289E-Ø7-Ø.2644912ØE-11-Ø.8Ø6Ø3Ø15E Ø4 Ø.12Ø4686E Ø2    Ø.ØØØØØØØØØ    4

C(GR)            J 3/78C  1.   Ø.   Ø.   Ø.S   3ØØ.ØØØ  5ØØØ.ØØØ    12.Ø11ØØ  1
 Ø.14324Ø54E Ø1 Ø.17555871E-Ø2-Ø.71889423E-Ø6 Ø.14Ø15Ø9E-Ø9-Ø.1ØØ69Ø94E-13    2
-Ø.68498756E Ø3-Ø.83936690E Ø1-Ø.39942Ø85E ØØ Ø.5Ø285536E-Ø2 Ø.33566391E-Ø6    3
-Ø.4716628ØE-Ø8 Ø.2351Ø115E-11-Ø.9918535ØE Ø2 Ø.14885486E Ø1     Ø.ØØØØØØØØ    4

H2O(L)           J 3/79H  2.O  1.   Ø.   Ø.L   273.15Ø   5ØØ.ØØØ    18.Ø152Ø  1
 Ø.2863Ø8ØØE Ø2-Ø.2Ø26Ø986E ØØ Ø.78529479E-Ø3-Ø.1365Ø2ØE-Ø5 Ø.91326966E-Ø9    2
-Ø.38579539E Ø5-Ø.11895046E Ø3 Ø.2863Ø8ØØE Ø2-Ø.2Ø26Ø986E ØØ Ø.78529479E-Ø3    3
-Ø.1365Ø2ØE-Ø5 Ø.91326966E-Ø9-Ø.38579539E Ø5-Ø.11895Ø46E Ø3     Ø.ØØØØØØØØ    4

KOH(L)          J12/7ØK  1.O  1.H  1.Ø  Ø.L   679.ØØØ  5ØØØ.ØØØ    56.1Ø56Ø  1
 Ø.99956469E Ø1     Ø.ØØØØØØØØ     Ø.ØØØØØØØØ     Ø.ØØØØØØØØ     Ø.ØØØØØØØØ    2
-Ø.52620731E Ø5-Ø.45334392E Ø2 Ø.99956469E Ø1     Ø.ØØØØØØØØ     Ø.ØØØØØØØØ    3
     Ø.ØØØØØØØØ     Ø.ØØØØØØØØ-Ø.52620731E Ø5-Ø.45334392E Ø2     Ø.ØØØØØØØØ    4
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ANNEX E to
STANAG 4400
(Edition 1)

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K2CO3(L)          J 3/66K  2.C  1.0  3.   Ø.L  1174.ØØØ  5ØØØ.ØØØ   138.2Ø58Ø  1
 Ø.25161469E Ø2     Ø.ØØØØØØØØ     Ø.ØØØØØØØØ     Ø.ØØØØØØØØ     Ø.ØØØØØØØØ    2
-Ø.14740138E Ø6-Ø.1311Ø73ØE Ø3 Ø.25161469E Ø2     Ø.ØØØØØØØØ     Ø.ØØØØØØØØ    3
     Ø.ØØØØØØØØ     Ø.ØØØØØØØØ-Ø.14740138E Ø6-Ø.1311Ø73ØE Ø3     Ø.ØØØØØØØØ    4

K2CO3(S)          J 3/66K  2.C  1.0  3.   Ø.S   3ØØ.ØØØ  1174.ØØØ   138.2Ø58Ø  1
 Ø.22824341E Ø2-Ø.13580993E-Ø1 Ø.8740989ØE-Ø5 Ø.11494425E-Ø7-Ø.67588149E-11    2
-Ø.14577844E Ø6-Ø.11Ø48665E Ø3 Ø.84398632E Ø1 Ø.18836256E-Ø1-Ø.46827483E-Ø6    3
-Ø.1Ø519610E-Ø7 Ø.64318412E-11-Ø.14166744E Ø6-Ø.34894424E Ø2     Ø.ØØØØØØØØ    4

K2S(L)            J 3/78K  2.S  1.   Ø.   Ø.L  1221.ØØØ  5ØØØ.ØØØ   11Ø.2566Ø  1
 Ø.12142927E Ø2 Ø.  Ø.ØØØØØØØØ     Ø.ØØØØØØØØ     Ø.ØØØØØØØØ     Ø.ØØØØØØØØ    2
-Ø.46520349E Ø5-Ø.54716Ø43E Ø2 Ø.12142927E Ø2     Ø.ØØØØØØØØ     Ø.ØØØØØØØØ    3
     Ø.ØØØØØØØØ     Ø.ØØØØØØØØ-Ø.46520349E Ø5-Ø.54716Ø43E Ø2     Ø.ØØØØØØØØ    4

END
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ATOMIC WEIGHTS AND CONSTANTS

The atomic weights, or relative atomic masses, of the elements listed below, and also the constants, are always subject to revision. The latest values produced by the IUPAC Commission on Atomic Weights as published in the journal "Pure and Applied Chemistry", or in the latest edition of the IUPAC publication "Quantities, Units and Symbols in Physical Chemistry" should be used. Note that the values used for the atomic weights will alter the values given in Annex E for the formula weights.

Table of Atomic Weights

Element	Atomic Weights
Aluminium	26.982
Barium	137.327
Carbon	12.011
Fluorine	18.998
Hydrogen	1.0079
Lead	207.2
Magnesium	24.305
Nitrogen	14.0067
Oxygen	15.9994
Potassium	39.0983
Sodium	22.9898
Sulphur	32.066

CONSTANTS

R, Universal gas constant = 8.314510 J/(mol-K)

TABLE OF FORMULAS AND ENTHALPIES OF PROPELLANT INGREDIENTS

Listed in the tables below are the enthalpies (heats) of formation for the main propellant ingredients used in gun propellants. To determine the thermochemical properties of propellants used in gun interior ballistics calculations the energies of formation are required. Using H=U+PV and assuming ideal gas behaviour then these can be obtained from the enthalpies of formation by the following formula

$$\Delta U_f = \Delta H_f - \Delta n\ R\ T$$

where

Δn - difference of mole numbers of gases at formation of the substance from the elements
R - gas constant (8.314510 J/(mol-K))
T - reference temperature (298.15K)
ΔU_f - energy of formation
ΔH_f - enthalpy of formation

and the PV product of condensed phases is neglected; it then follows that

$$U_f^\circ = \Delta U_f^\circ - (PV)_{reactants}$$

The values of the thermochemical properties to be calculated are strongly dependent on the enthalpies of formation used. These values can vary considerably from source to source. The data tabulated below was extracted from "Heats of Formation of Components for Rocket Propellants, Gun Propellants and High Explosives" by Volk, F. and Bathelt, H., Fraunhofer-Institut Fur Chemische Technologie, T/RF 11/K 0001/K 1100, January 1990. Data for propellant ingredients not listed below should be taken from this report. If not then the source of the enthalpy of formation should be given.

Ingredient	Formula									Enthalpy of formation (kJ/mol)
Nitrocellulose, 11.00 %N	C	6.	H	8.031	O	8.939	N	1.969		-756.13
Nitrocellulose, 11.10 %N	C	6.	H	8.003	O	8.994	N	1.997		-753.37
Nitrocellulose, 11.20 %N	C	6.	H	7.975	O	9.050	N	2.025		-750.53
Nitrocellulose, 11.30 %N	C	6.	H	7.946	O	9.107	N	2.054		-747.68
Nitrocellulose, 11.40 %N	C	6.	H	7.918	O	9.165	N	2.082		-744.79
Nitrocellulose, 11.50 %N	C	6.	H	7.889	O	9.223	N	2.111		-741.91
Nitrocellulose, 11.60 %N	C	6.	H	7.859	O	9.281	N	2.141		-738.94

Ingredient	Formula	Enthalpy of formation (kJ/mol)
Nitrocellulose, 11.70 %N	C 6. H 7.830 O 9.340 N 2.170	-735.97
Nitrocellulose, 11.80 %N	C 6. H 7.800 O 9.400 N 2.200	-732.99
Nitrocellulose, 11.90 %N	C 6. H 7.770 O 9.460 N 2.230	-729.94
Nitrocellulose, 12.00 %N	C 6. H 7.739 O 9.521 N 2.261	-726.89
Nitrocellulose, 12.10 %N	C 6. H 7.709 O 9.583 N 2.291	-723.79
Nitrocellulose, 12.20 %N	C 6. H 7.677 O 9.645 N 2.323	-720.65
Nitrocellulose, 12.30 %N	C 6. H 7.646 O 9.708 N 2.354	-717.51
Nitrocellulose, 12.40 %N	C 6. H 7.614 O 9.772 N 2.386	-714.29
Nitrocellulose, 12.50 %N	C 6. H 7.582 O 9.836 N 2.418	-711.07
Nitrocellulose, 12.60 %N	C 6. H 7.549 O 9.901 N 2.451	-707.81
Nitrocellulose, 12.70 %N	C 6. H 7.517 O 9.967 N 2.483	-704.50
Nitrocellulose, 12.80 %N	C 6. H 7.483 O 10.033 N 2.517	-701.15
Nitrocellulose, 12.90 %N	C 6. H 7.450 O 10.100 N 2.550	-697.81
Nitrocellulose, 13.00 %N	C 6. H 7.416 O 10.168 N 2.584	-694.38
Nitrocellulose, 13.10 %N	C 6. H 7.382 O 10.237 N 2.618	-690.95
Nitrocellulose, 13.20 %N	C 6. H 7.347 O 10.306 N 2.653	-687.43
Nitrocellulose, 13.30 %N	C 6. H 7.312 O 10.376 N 2.688	-683.92
Nitrocellulose, 13.40 %N	C 6. H 7.276 O 10.447 N 2.724	-680.36
Nitrocellulose, 13.50 %N	C 6. H 7.240 O 10.519 N 2.760	-676.76
Nitrocellulose, 13.60 %N	C 6. H 7.204 O 10.592 N 2.796	-673.12
Nitrocellulose, 13.70 %N	C 6. H 7.167 O 10.665 N 2.833	-669.40
Nitrocellulose, 13.80 %N	C 6. H 7.130 O 10.740 N 2.870	-665.67
Nitrocellulose, 13.90 %N	C 6. H 7.093 O 10.815 N 2.907	-661.91
Nitrocellulose, 14.00 %N	C 6. H 7.055 O 10.891 N 2.945	-658.10
Nitrocellulose, 14.10 %N	C 6. H 7.016 O 10.968 N 2.984	-654.21
Nitrocellulose, 14.14 %N	C 6. H 7.000 O 11.000 N 3.000	-652.66
Acetone	C 3. H 6. O 1.	-248.11
Akardite 2	C 14. H 14. O 1. N 2.	-106.69
Ammonium nitrate	H 4. O 3. N 2.	-365.14
Barium nitrate	O 6. N 2. Ba 1.	-991.86
Calcium carbonate	C 1. O 3. Ca 1.	-1206.96
Cellulose diacetate	C 10. H 14.069 O 7.035	-1374.86
Cellulose triacetate	C 10. H 13.290 O 6.586	-1325.49
Decalin	C 10. H 18.	-230.71
Dibutyl phthlate	C 16. H 22. O 4.	-842.66
Diethyleneglycol dinitrate (DEGDN)	C 4. H 8. O 7. N 2.	-415.89

Ingredient	Formula	Enthalpy of formation (kJ/mol)
1,1-dimethyl hydrazine (UDMH)	C 2. H 8. N 2.	+49.79
2,4-dinitro-diphenylamine (NNDP)	C 12. H 9. O 4. N 3.	+22.59
2,4-dinitrotoluene	C 7. H 6. O 4. N 2.	-71.55
2,3-dinitrotoluene	C 7. H 6. O 4. N 2.	-15.90
2,5-dinitrotoluene	C 7. H 6. O 4. N 2.	-34.31
2,6-dinitrotoluene	C 7. H 6. O 4. N 2.	-51.13
3,4-dinitrotoluene	C 7. H 6. O 4. N 2.	-14.64
3,5-dinitrotoluene	C 7. H 6. O 4. N 2.	-43.51
Diphenylamine	C 12. H 11. N 1.	+116.86
Diphenylurethane	C 15. H 15. O 2. N 1.	-338.07
Ethanol	C 2. H 6. O 1.	-277.90
Ethyl centralite (carbamite)	C 17. H 20. O 1. N 2.	-105.02
Ethylenediamine dinitrate	C 2. H 10. O 6. N 4.	-651.87
Ethylene glycol	C 2. H 6. O 2.	-454.93
Ethylphenylurethane	C 11. H 15. O 2. N 1.	-463.59
Glycerin	C 3. H 8. O 3.	-668.60
Hexogen (RDX)	C 3. H 6. O 6. N 6.	+66.53
Hydrazine	H 4. N 2.	+50.63
Hydrazine nitrate	H 5. O 3. N 3.	-251.58
Hydroxylammonium nitrate	H 4. O 4. N 2.	-344.76
Isopropylammonium nitrate	C 3. H 10. O 3. N 2.	-414.22
Methriol trinitrate	C 5. H 9. O 9. N 3.	-443.50
Methyl centralite	C 15. H 16. O 1. N 2.	-61.09
Nitric acid	H 1. O 3. N 1.	-173.47
2-nitro-diphenylamine	C 12. H 10. O 2. N 2.	+64.43
Nitroglycerin	C 3. H 5. O 9. N 3.	-370.70
Nitroguanidine	C 1. H 4. O 2. N 4.	-92.88
Octogen (HMX)	C 4. H 8. O 8. N 8.	+75.02
Pentaerylthritol tetranitrate (PETN)	C 5. H 8. O 12. N 4.	-538.90
Potassium nitrate	O 3. N 1. K 1.	-492.71
Potassium sulfate	O 4. S 1. K 2.	-1433.86
Sodium aluminium fluoride (cryolite)	Na 3. Al 1. F 6.	-3301.18
Sodium nitrate	O 3. N 1. Na 1.	-467.44

Ingredient	Formula	Enthalpy of formation (kJ/mol)
Triacetin	$C_9H_{14}O_6$	-1330.93
Triethyleneglycol dinitrate	$C_6H_{12}O_8N_2$	-606.68
Trimethylammonium nitrate (TMAN)	$C_3H_{10}O_3N_2$	-305.85
Water	H_2O_1	-285.85

SUMMARY OF PROPELLANT CHARACTERISTICS

PROPELLANT NUMBER:_____ INFORMATION SUBMITTED BY:_____

COUNTRY OF ORIGIN:_____ NAME:_____

MANUFACTURER:_____ ACTIVITY:_____

DESIGNATION OF DATE:_____

COMPOSITION:_____ _____

SPECIFICATION:_____

1. TYPE OF PROPELLANT:_____ 2. METHOD OF MANUFACTURE:_____

_____ _____

(solvent-extruded, rolled, etc)

3. INTENDED USE:_____ 4. OTHER RELATED COMPOSITION:_____

_____ _____

5. LOADING DENSITY:_____

6. COMPOSITION:

CONSTITUENT	% BY MASS Nominal ±TOLERANCE	OTHER INFORMATION
Nitrocellulose		N% of NC:
Total Volatiles		

Total Moisture		
Residual Solvent		
Ash		

7. STABILITY TESTS: (STANAG 4117 and Other Methods)

TEMP.°C	METHOD USED	RESULTS	REQUIREMENTS	REFERENCE

PROPELLANT NUMBER:_____

8. HEAT OF EXPLOSION (Q):_____J/kg _____J/kg
(At 25°C, H_2O Liquid (Experimental) (Calculated)
METHOD OF CALCULATION:_____

9. DENSITY OF SOLID PROPELLANT:_____kg/m³

10. ISOCHORIC ADIABATIC FLAME TEMPERATURE (Tv):_____K
METHOD OF CALCULATION: _____

11. MOLES/kg OF GAS AT ISOCHORIC FLAME TEMPERATURE (n):_____
METHOD OF CALCULATION: _____

12. RATIO OF "FROZEN" SPECIFIC HEATS FOR
PROPELLANT GASES (Cp/Cv)_____AT_____K
METHOD OF CALCULATION: _____

3. FORCE (f_p):_____J/kg

METHOD OF CALCULATION:_____

1

4. COVOLUME (η):_____m^3/kg

METHOD OF CALCULATION:_____

15. COMBUSTION PRODUCTS:

COMPONENT	AT K	mol/kg

METHOD OF CALCULATION: _____

16. BURNING RATE (Obtained by Strand Burner, Closed Vessel, etc)

r=_____m/s valid at _____°C from p_____to_____Pa

r=_____m/s valid at _____°C from p_____to_____Pa

r=_____m/s valid at _____°C from p_____to_____Pa

17. REMARKS AND OTHER INFORMATION:

SELECTED BIBILOGRAPHY

1.	Bac J P	Bagheera, A Ballistic Thermodynamic Code, 3rd International Gun Propellant Symposium, Picatinny Arsenal, Dover, New Jersey, 30 Oct-1 Nov 1984,
2.	Hunt F R W (Editor)	Internal Ballistics, HMSO, 1951.
3.	Corner J	Tables of Pressure-Corrections in the Thermochemistry of Propellant Explosions, ARD Theoretical Research Report 8/43, Dec 1943.
4.	Corner J	The Derivation of Pressure-Corrections in the Thermochemistry of Propellant Explosions, ARD Theoretical Research Report 9/43, Dec 1943.
5.	Pike H H M	Thermochemical Data for Propellant Ingredients and their Products of Explosion, ARE Theoretical Research Report 4/49, Dec 1949.
6.	IUPAC Commission on Atomic Weights	Atomic Weights of the Elements Pure and Applied Chemistry 1972, 30, p639-649.
7.	Jacquemin P Nicolas M	Calcul des Performances Thermodynamiques des Poudres aux Hautes Densites de Chargement, Proceedings of the 5th International Symposium on Ballistics, France 1980.
8.	Longdon L W (Editor)	Textbook of Ballistics and Gunnery, Volume 1, HMSO, 1987.
9.	Stiefel L (Editor)	Gun Propulsion Technology, Volume 109 in AIAA Progress in Astronautics and Aeronautics Series, 1988.
10.	Chase M W (Editor)	JANAF Thermochemical Tables, Journal of Physical Chemistry Reference Data, Vol 14, Suppl. 1, 1985.
11.	Corner J	Theory of the Interior Ballistics of Guns, John Wiley & Sons, Inc, 1950.

12. Press W H
Flarmery B P
Tenkolsky S A
Vetterling W T
Numerical Recipes, The Art of Scientific Computing. Cambridge University Press, 1986.

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

14. Zeleznik F J
Gordon S
NASA Technical Note D-473, An Analytical Investigation of Three General Methods of Calculating Chemical Equilibrium Compositions, 1960.

15. Zeleznik F J
Gordon S
Calculation of Complex Chemical Equilibria, Ind Eng Chem, Vol 60, No 6, pp27-57, June 1968.

16. Gordon S
McBride
NASA SP273 Interim Revision 1976, Computer Program for Calculation of Complex Chemical Equilibrium Compositions, Rocket Performance, Incident and Reflected Shocks and Chapman-Jouguet Detonations, 1976.

17. Gill P E
Murray W
Wright M H
Practical Optimisation, Academic Press, 1981.

18. Sutterlin R
Cours de Munitions, Livre II, Physique des Explosifs Tome II, 1964.

19. Vidart A
Laboratoire de la Commission des Substances Explosives Calcul des Caracteristiques des Explosifs Condenses, 1960.

20. Corner J
Tavernier M P
Balistique Interieure Theorique, Resume et Adaptation de "Theory of Interior Ballistics of Guns", 1956.

21. Corner M J
Proprietes Thermodynamiques des Produits de la Combustion sous haute Pression, M.A.F. Tome 26. 3e Fascicule 1952.

22. Krier H
Summerfield M
Interior Ballistics of Guns, Vol 66 of AIAA Progress in Astronautics and Aeronautics, 1979.

22a. Krier H
Summerfield M
Balistique Interieure des Canons, p380, Translation SNPE/CRB sous la direction de B Zeller, 1984.

23. Volk F
Bathelt H
Propellants & Explosives 1,p7-14(1976), Application of the Virial Equation of State in Calculating Interior Ballistics Quantities, 1976.

24. Daree K
Coefficients du Viriel et Potentiel Intermoleculaire, Rapport ISL R102/84, 1984.

25. Jacquemin P
Nicolas M
Calcul des Performances Thermodynamiques des Poudres aux Hautes Densites de Chargement, SNPE/CRB N.T. No. 66/80/CRB/NP, 1980.

26. Jacquemin P
Programme ONYX: Description Theorique et Informatique, SNPE N.T. No. 26/82/CRB/NP, 1982.