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# Computer Program for Internal Aluminum-Fuel-Air Explosions

by  
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AUGUST 1983

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## FOREWORD

This report documents the extension of the continuing research effort on internal blast at the Naval Weapons Center to include aluminized fuels in air. Work was performed during the period 1978-1982.

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(U) This report documents the internal explosion computer program INAL, used to calculate overpressures, temperatures, and chemical species present in the internal explosion of aluminized fuels in air. A complete listing of the program in HP-BASIC is presented, as well as a discussion of the function performed in each major subroutine.

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## INTRODUCTION

This report describes a program used to calculate overpressures in internal explosions of aluminized fuels in air. The program, formerly called INE, has been slightly modified and is called *INAL* (internal explosions with aluminum). An annotated copy of the *INAL* program appears in Appendix A.

The calculations are based on the assumptions that the process as a whole is adiabatic, that the products are uniformly distributed through the volume, that chemical and thermal equilibria prevail, and that the ideal gas law may be used throughout. The adiabatic assumption in a constant volume system is equivalent to the requirement that there be no net change in internal energy; that is, that the internal energy of the products (34 chemical species are considered) must be equal to that of the introduced fuel (inasmuch as all the other starting materials are elements in their thermochemical reference states).

A description of the program can rather logically be divided into two segments: (1) the main program, in which the general procedure is to find, by trial and error, a product temperature for which the adiabatic condition holds; and (2) the subroutine, called *Alcal*, which carries out the equilibrium calculations and then finds the internal energy change corresponding to the equilibrium set of products.

## MAIN PROGRAM

### INPUT SECTION

*Fuel.* enter formula and internal energy of formation. Computes formula mass; allows for zero C or H or no fuel.

*Conc* (accessible from line 1780) resets flags, counters, and amounts of solids to zero. Enter concentration ( $\text{kg/m}^3$ ) of fuel and of Al. Computes moles of fuel and of atoms of Al, C, H, N, O. Computes total initial internal energy.

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*Temp* (for entering trial temperature manually) may be accessed by use of special function key *k4*. After at least two trials, *Temp* may be bypassed and interpolation used to find the new temperature.

### COMPUTATION SECTION

*Calc* calls up the computational subroutines *Eq*, *Alcal*, and *Ex*.

*Eq* is a subroutine of the main program to evaluate equilibrium constants of formation of each of the 34 chemical species.  $K_p$  is first computed from the stored parameters and then converted to  $K_n$  (expressed in mole numbers).  $K_p$  is defined for each chemical species as the ratio of the activity of the species to the product of the activities of C, Al vapor,  $H_2$ ,  $N_2$ , and  $O_2$ , each raised to the power corresponding to the stoichiometric content of the element. In converting the  $K_p$ , the activities of gaseous species, including the elements, are changed to mole numbers. For the condensed species the standard state remains the pure phase, so that the activity is unity, except for C.<sup>1</sup>

*Alcal* is the master subroutine which carries out equilibrium and energy calculations. Results are displayed as "dU" (net) and "T high" or "T low"; dU = 0 is desired for convergence. A new temperature approximation is performed automatically by interpolation, based on former T and dU values; or else it is entered manually with *k4*.

*Ex* prepares termination of calculation. Calls up *Molsum*, finding the total moles of gases.

### OUTPUT

Prints results of calculations.

$C_v$ , the molar heat capacity at constant volume, is computed by finding dU at  $t_{\cdot}$  nearby temperatures. An isentropic parameter, lambda, is found by using also  $dn/dT$  (change of mole number of gas with temperature).

Conclusion: various options allowed, as for new concentrations or a new fuel.

<sup>1</sup> Naval Weapons Center. *Adiabatic Computation of Internal Blast from Aluminum-Cased Charges in Air*, by R. A. Reinhardt and A. K. MacDonald, Naval Postgraduate School, China Lake, Calif., NWC, January 1982. (NWC TP 6257, publication UNCLASSIFIED.)

## ALCAL SUBROUTINE

*Alcal* is the major computational subroutine whose task is to find the numbers of moles of the products present at equilibrium at the selected temperature. The conditions to be satisfied (other than for the trivial case of Ar) are the atom balance conditions for C, H, N, O, and Al and the establishment of chemical equilibrium between each compound and its component elements in their reference states at the prevailing temperature.

The master variables (all in mole numbers) are  $X = \sqrt{O_2}$ ,  $Y = \sqrt{H_2}$ ,  $Z = \sqrt{N_2}$ ,  $Al_v$  = Al metal vapor,  $Acc$  = activity of C (standard state = graphite). Of these,  $Y$  is always computed in closed form; from one to four of the remaining master variables are found as unknown parameters, using the Newton-Raphson method. The actual number of unknowns is equal to four, reduced by the number of condensed phases present. Possible condensed phases are:  $Al_2O_3$  (solid or liquid), Al (liquid), AlN (solid), C (solid),  $Al_4C_3$  (solid). The presence or absence of each condensed phase is indicated by a flag, to be set as described later. The set of condensed phases is referred to as a *regime*; allowance is made in the program for about 20 different regimes.

Based on the values of the master variables and the  $K_n$  of formation, the mole number of each species is computed. Then the material balance in the elements O, N, C, and Al is written in terms of these mole numbers. Thus, there results a set of up to four simultaneous non-linear equations. It is this set which is used as the basis of the Newton-Raphson scheme to find the unknown parameters.

At the conclusion of an iteration, the newly generated values of the master variables are used to repeat the calculations. In favorable situations each iteration results in improvement (although temporary divergence sometimes occurs). Iteration is repeated until errors in the material balances are less than one part in ten thousand.

## INITIAL APPROXIMATION

To begin the calculation, an initial approximation of the master variables is made using the subroutine *Approx*. In this approximation an arbitrary hierarchy of oxygen and nitrogen uptake is assumed. Oxygen is assumed to produce, in order, CO,  $Al_2O$  (g),  $Al_2O_3$  (c),  $H_2O$ ,  $CO_2$ , and  $O_2$ . When there is insufficient O to convert all Al to  $Al_2O_3$ , AlN is assumed present. If there is not sufficient O to convert all C to CO,  $Al_4C_3$  is considered if the temperature is low enough. This rather long subroutine has given many more satisfactory initial conditions than the simpler scheme described in Reference 1. It is used once, or at most twice, for each new concentration that is run.

REGIMES IN *ALCAL*

It is necessary to assume which condensed phases are present, then perform the calculations previously outlined, and finally test for the presence of the condensed phases. The following criteria must be met: (1) the quantity of the phase must be positive and (2) the formation constant must be satisfied. The tests are carried out after the convergence of the Newton's method calculation. If the tests fail, a different regime (set of condensed phases) is tried--the assumptions now based on the currently computed sets of mole numbers.

An index *Nw* is used to identify the regime being considered. Eleven different values of *Nw* are allowed, which account for about 20 different regimes, since for most values of *Nw* graphite may be present or absent. A key to the *Nw* values is given at the end of the program in Appendix A.

LABEL *HOM*

The section of *Alcal* beginning at label *Hom* is the setup for the Newton's method calculation. (*Hom0* is merely an early entrance into *Hom*.) Depending on the regime selected, *li* (the number of variables) and *Nw* (the index identifying the regime) are evaluated by the subroutines *liset* and *Nwset*. The regime is established in a variety of ways. Initially, *Approx* gives the first guess. Afterwards, the subroutine *Alntest* is used as criterion for all solids except  $Al_4C_3$ , which is looked for at *Hom2*. At *Exit* and *Exit1* additional tests for alumina and graphite are made.

The various subdivisions of *Hom* are designated *Nwx*, where *x* is partly indicative of the value of *Nw* for the regime considered. The correspondence is imperfect since *Nw1* includes the cases of *Nw* = 1, 4, and 5 and *Nw2* includes *Nw* = 2 and 6. In each case, initial approximations are set for each variable to be solved, using latest results of the appropriate variable.

Subroutine *Newt* is called to carry out the calculations (except *Nw* = 4, for which solution in closed form is possible). Then either a new value of *Nw* is used (as called for by *Alntest* and *liset*) or the program switches to *Hom2*. At this point, if  $Al_4C_3$  had not been presupposed, but was found present, it is necessary to pass once again through *Approx*. Otherwise exit from the subroutine is prepared.

EXIT FROM *ALCAL*

At *Exit* and *Exit1* it is necessary to check for negative amounts of alumina and graphite. If found, the appropriate flags must be reset and a return to *Hom* is required. If those tests are satisfactory, next, at label *Energy*, the internal energy, for each species is calculated making use of the stored parameters and the number of moles of the species. If  $T = 2315$  K (the melting point of alumina), the relative

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amounts of the two phases of alumina are found from the energy balance. Return to the main program then takes place.

### SUBROUTINES IN *ALCAL*

*Alntest* sets flags for AlN, Al<sub>2</sub>O<sub>3</sub>, Lq (= liquid Al), and Gr (graphite) based on the present value of the formation expression, as related to the formation constant for the first three, and on whether *Acc* has been found less than unity (indicating no graphite).

*Iiset* and *Nwset* evaluate *Ii* (the number of variables to be solved for) and *Nw* (the index for the solids regime), based on the flags set by *Alntest*.

*Newt* solves the set of simultaneous non-linear equations needed to find the values of the master variables, using the Newton-Raphson method.

*Fx* gives the fitting functions for *Newt*. The subdivisions are labelled *Fxy* where *y* is a value appropriate to that of *Nw*. The subroutine generates a variable designated *Fx* (returned to *Newt*), which gives the fractional error in the stoichiometry for whichever element is being considered at the moment. Since *Fx* calls on *Spec*, mole numbers of all species are found each time.

*Diff* first computes all the master variables which were not found in *Fx* and then calls *Spec* to find all the mole numbers of the gaseous species. *Diff* computes mole numbers of the condensed species; and finally the errors in the material balances for O, N, Al, and C are returned to *Fx*.

*Spec* computes the mole numbers of all gaseous species, given the current values of *X*, *Z*, *Alv*, and *Acc*.  $Y = \sqrt{H_2}$  is computed in closed form in *Spec*; it is needed for computations on the hydrogen-containing species. For each species the mole number is computed by using appropriate values of *K<sub>n</sub>*, the formation constant.

### DIAGNOSTIC SUBROUTINES

*Sum1* is called at the end of each run to give first a check on the material balance in each element and then, at *Testk*, a comparison of the computed amounts with the equilibrium constants of formation of each condensed phase and of several key gaseous species.

*Printt* is called whenever special function key *k0* has been depressed once. At each emergence from *Newt* the mole numbers of all species are given in a condensed table, this is followed by *Sum1* and *Testk*, which give output as previously described. These various checks are especially valuable in troubleshooting.

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Depressing special function key *kI* will cause execution of TRACE VARIABLES  $Y_n(*)$ . Then during each iteration in *Newt* the relative error functions, used to test convergence, will be displayed. Each  $Y_n(J)$  must drop below 0.0001 in absolute value before convergence is realized. This feature may be turned off by executing NORMAL.

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## Appendix A PROGRAM INAL

This program is written in Hewlett-Packard's HP-BASIC, and is intended for use on any of the HP 9845 series computers. In addition to the main program, the data file "THD" and the key file "INEK" are needed for operation.

### KEY FILE INEK

KEY 0  
Check-(Check-0)  
-Execute

KEY 1  
TRACE VARIABLES Yn(\*)  
-Execute

KEY 2  
CONT Er  
-Execute

KEY 3  
RE-STORE ==  
-Left arrow  
-Insert character

KEY 4  
CONT Temp  
-Execute

KEY 5  
TRACE PAUSE Iiset  
-Execute

KEY 6  
TRACE PAUSE S  
-Execute

KEY 7  
7,5,3,6  
-Continue

KEY 8  
CONT Fuel  
-Execute

KEY 9  
-Clear line  
LOAD

KEY10  
-Clear line  
SAVE

KEY11  
-Clear line  
STORE

KEY12  
-Clear line  
EDIT

KEY13  
-Clear line  
EDIT LINE

KEY14  
-Clear line  
LIST

KEY15  
-Clear line  
SCPATCH

KEY16-Undefined  
KEY17-Undefined  
KEY18-Undefined  
KEY19-Undefined  
KEY20-Undefined  
KEY21-Undefined  
KEY22-Undefined  
KEY23  
-11750  
-Continue

KEY24-Undefined  
KEY25-Undefined  
KEY26-Undefined  
KEY27-Undefined  
KEY28-Undefined  
KEY29-Undefined  
KEY30-Undefined  
KEY31-Undefined





```

1330 Ceev1: U1=DU
1340 U1=DU
1350 NAT(1)=Deltfactor)NT1
1360 COSUB EG
1370 COSUB A1CAL
1380 U2=DU
1390
1400 Ceev2: PRINT "Deltfactor=";Deltfactor
1410 PRINT "FOR C=1 TO 10 IN COSUB PRINT"
1420 IF C(1)=1 THEN Ceev1
1430 IF (N(1)) THEN EXPR(AE(1,2)) TO "N(1);SPA(2)";
1440 PRINT F(1); " CHANGES FROM ";N(1); " TO ";N(1);SPA(2)
1450 NEXT Y
1460 Dn_dt=(Nsum-Ng)/Deltfactor/T
1470 Ceev=(U2-U1)/Deltfactor/T
1480
1490
1500 Ceep: Lambda=(Ng+T*Dn_dt)*B.314/Ceev
1510 Ceep=Ceev/Ng THEN Ceep2
1520 PRINT "dn/dt=";Dn_dt;" Cv=";Cv;" nsum=";Nsum;" N(1)"; "Ng;LIN(1); "U1=";U1;" U2=";U2;"-1.-2
1530 STANDARD
1540
1550 Ceep2: Branch=3
1560 IF Deltfactor<0 THEN Ceep3
1570 C=0
1580 INPUT "DO YOU WANT TO REPEAT FOR dV AND dt NEGATIVE (Y/N)?" ;Cs
1590 IF C(1)=Y THEN Ceep3
1600 Deltfactor=-.001
1610 Ceep=Ceev
1620 Ceep2
1630 Ceep3: Imce=Lambda/Ceev
1640 PRINT "Using Imce=";Imce;" Cv r " ;3D.3D;" J/K/Kg"
1650 Imcf: Imce=Imce*Lambda/Ceev
1660 PRINT "Using Imcf=";Imcf;" Overpressure r = 3D.3D;" bars". " Volume r " ;3D.3D;" cu m"
1670 PRINT USING Imcf;" PAGE "
1680 PRINT "LIN(4);PAGE "
1690 INPUT "DO YOU WISH TO RUN ANOTHER CONCENTRATION FOR THIS SAME METAL--FUEL PAIR (Y/N)?" ;Cs
1700 IF C(1)=Y THEN Ceep3
1710 INPUT "DO YOU WISH TO RUN A DIFFERENT FUEL WITH THE SAME METAL (Y/N)?" ;Cs
1720 PRINT "END OF ROUTINE"
1730 STOP
1740
1750
1760
1770
1780
1790
1800
1810
1820
1830
1840
1850
1860
1870
1880
1890
1900
1910
1920
1930

```

Saving the original values

For Cv calcul.

! Either both 0 or both >0

! Cons; U

! per unit mass

! Ng;LIN(1); "U1=";U1;" U2=";U2;"-1.-2

! Computes Kn FROM LGT(Kp) parameters  
 Kn is equal. const. of formation from elements.  
 UNIT FOR CONST VOL = 0.001 CU M.

! Conversion from Kn (expressed in pressures) to Kn.  
 An(I,2) avoids overflown in Kp  
 AN(I,2) is delta n (gasus) for formation reaction.  
 AN(I,2) not used



Excess of N over Al

AlN absent, alumina present

H2O assumed absent

Alumina and Al2O both at 1.2600  
These two eqns satisfy the Al and O balances  
Equil. with Al2O and alumina

Equil. with CO and O2

Equil. with O2 and Al2O

H2O present

CO2 absent

These 2 eqns satisfy the H, and O balance.  
Equil. of O2 with H2O and H2  
Equil. with CO and O2  
Equil. with O2 and alumina

CO2 and H2O present

O2 assumed absent

Carbon balance

Equil. with CO and CO2

Prepare eqns from approx

CO absent

Except O2

Equil. with CO2 and O2

Equil. with O2 and alumina

End of approximations

```

2440 Excn2: Al=Al*(100*Na1-2*(Na0-Nc))
2450 Al=N*(N2/n)/2
2460 Al=M*(1/2)/K(20)
2470 Lqflag=Lq=0
2480 X=Al2o/Alv*(K(4)
2490 IF T(500) THEN X=Alv*(-2/3)*Kao*(-1/3)
2500 GOTO Prep1
2510 Nealn=Nu*1
2520 AlnLq=Gr-Alnflag=Lqflag=0
2530 Al=Al
2540 I=1
2550 N2=NH/2
2560 Z=SOR(N2)
2570 IF Nea-Nc > 1.5*Na1 THEN Water
2580 C=NC
2590 Aa=(Na0-Nc-Na1)/2
2600 O2=K(A)/Kao/Al2o
2610 Y=SOR(O2)
2620 H2=NH/2
2630 Y=SOR(H2)
2640 Alv=M*SOR(Al2o/X/K(1))
2650 GOTO Hom
2660 Water: A=Na1/2
2670 IF Nea-Nc > 1.5*Na1+NH/2 THEN Carbd
2680 B=NH
2690 H2=NH/2-Na+NC+1.5*Na1
2700 X=H2o/H2/K(12)
2710 Prep2: Acc=Co/X/K(7)
2720 M=Alv*SOR(1/X*3/Kao)
2730 GOTO Hom
2740 Carbd: H2o=NH/2
2750 IF Nea > 1.5*Na1+NH/2 THEN Oxy
2760 C=Na0-Nc-1.5*Na1-NH/2
2770 CompC=Co2/Co/K(8)
2780 GOTO Prep2
2790 Oxy: Co2=NC
2800 C=C*(Na0-Nc-1.5*Na1-NH/2)/2
2810 X=SOR(O2)
2820 Acc=Co2/O2/K(8)
2830 M=Alv*SOR(1/X*3/Kao)
2840 GOTO Hom
2850
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```





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Variable is A1v; Num10; A1cflag=2;  
 Alumina; A1n; A1c plus excess A1

If any change then recompute  
 Avoids material balance errors

Variables are A1v, Z1; A1cflag=2; Num11;  
 Alumina; A1c plus excess A1  
 Phase rule requirement

If any change then recompute  
 These two to avoid material balance problems

```

4520 Num10; REBIN Xn(1) ;
4530
4540 GOTO Num10
4550 GOTO Num10
4560 GOTO Num10
4570 GOTO Num10
4580 GOTO Num10
4590 GOTO Num10
4600 GOTO Num10
4610 GOTO Num10
  
```

```

4620 Num11; REBIN Xn(2) ;
4630
4640 GOTO Num11
4650 GOTO Num11
4660 GOTO Num11
4670 GOTO Num11
4680 GOTO Num11
4690 GOTO Num11
4700 GOTO Num11
4710 GOTO Num11
4720 GOTO Num11
4730 GOTO Num11
4740 GOTO Num11
  
```











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```

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9440 | .....
9450 | .....
9460 | .....
9470 | .....
9480 | .....
9490 | .....
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9560 | .....
9570 | .....
9580 | .....
9590 | .....
9600 | .....
9610 | .....
9620 | .....
9630 | .....
9640 | .....
9650 | .....
9660 | .....
9670 | .....
9680 | .....
9690 | .....
9700 | .....
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9720 | .....
9730 | .....
9740 | .....
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9780 | .....
9790 | .....
9800 | .....
9810 | .....
9820 | .....
9830 | .....
9840 | .....
9850 | .....
9860 | .....
9870 | .....
9880 | .....
9890 | .....
9900 | .....
9910 | .....
9920 | .....
9930 | .....
9940 | .....
9950 | .....
9960 | .....
9970 | .....
9980 | .....
9990 | .....
1000 | .....

```

Input: X,Kaa  
Al upper

INPUT: Aicflap, Ncc + Acc IF Aic Is present  
Graphite assumed absent

No Graphite for this case  
Limiting activity of C(c)  
If Aicflap, Acc=0 must be carried back to Next

INPUT: Z=SQR(N2), Ncc, Acc  
Coefficients of nonhydrogen species  
Complete atom balance in H, Y=SQR(H2)

Corrected moles of N atoms  
Corrected atom balance in C





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DATA FILE THD

1. Equilibrium Constant of Formation Data

0	0	0	0	0	0
-2.04642317215	3095.08563709	-61.4431030074	-7.59713579400E-05	2.49078062430E-03	-.5
-6.02750724995	26914.0692052	1.94410164793	9.72325196131E-06	9.52727405371E-05	-1
-0.50206579927	40170.5376063	-0.77650900461	-1.74973054021E-04	4.90920260606E-03	-.5
2.25546550767	-32795.0697374	27.3534102517	9.00703939722E-05	2.37493930912E-03	1
0	0	0	0	0	0
4.59311031464	6100.44304152	29.700241155	-6.72129593009E-05	9.17169097642E-05	.5
6.74063151113E-02	20641.664597	1.10073929201	-2.43670722090E-05	6.32400077623E-05	0
3.13209970797	-12016.3695425	19.0339617644	1.40157371394E-05	0.41355776673E-05	.5
.769405272297	-1960.95209501	-16.3430133692	-1.47402301947E-05	4.41263920063E-05	0
0	0	0	0	0	0
-3.05603740471	13305.1920091	13.0679740254	-5.19032403354E-06	4.75004033074E-05	-.5
-2.94319764443	12909.3260156	5.26330004125	6.70630394752E-05	1.05115930504E-04	-.5
-6.14764405566	26105.034292	-7.41170320136	1.04032404614E-05	1.16220007003E-04	-1
.710103195616	-4000.04503459	7.7034272203	-9.00440254772E-06	3.52020067050E-05	0
0	0	0	0	0	0
3.49713046375	-13430.7266053	9.70006100770	6.17322760660E-06	6.93355557051E-05	.5
0	0	0	0	0	0
-5.95275504025	15650.2501090	-20.0673104972	9.04206100206E-05	1.71621469196E-04	-1
-10.9363510792	31054.2661256	-37.261473539	-1.17310000542E-04	2.75106302573E-03	-.5
-40.6069700932	154372.094779	202.327462644	1.92799147057E-03	6.13052065702E-03	-3.5
-29.4359333294	110007.365935	-6.00469062004	5.06473330935E-04	3.13010000764E-04	-3.5
0	0	0	0	0	0
.025767716905	4.76032635592	-2410.34572094	4.65494992401E-05	1.61047243700E-02	-.5
5.09215003192	-22210.0465015	-11.9501155333	-1.64335070309E-05	2.07761703011E-04	.5
6.52930290135	-24260.9161704	-12.4711153722	-4.29703319993E-05	1.06617359720E-04	.5
7.0602273036	-29343.3317977	-.370425411396	-6.61291975014E-05	9.54771077177E-05	.5
-24.9026257077	71142.0930524	-49.1302110137	-5.19454632333E-04	6.46607977746E-03	-4
1.60731167515	-6006.70452602	-12.0660091672	-7.69075947010E-06	5.53906500107E-05	0
-25.7403753901	96490.0463919	2562.02767313	2.06105217604E-03	1.15261013721E-02	-.5
2.2214151064	1209.01995973	219.335325609	-5.99683071430E-05	4.36611516909E-05	0
-2.03590036359	0769.63261573	10.2050441719	-1.62155531526E-05	9.66245762320E-05	-.5
2.65401667607	-11332.2620300	-15.5572440176	1.36720709929E-07	6.45226563072E-05	0
10.0495007765	-41395.0614497	-16.0531546361	-1.05667525960E-04	3.09781110914E-04	1

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2. Internal Energy of Formation Data

310931.276915	11.6599712	.00007516556	1364.27600	664251.04
264015.420609	30.1511592	.00027214828	-2961.0168	1039598.40
-55065.7557	60.797312	-.0003553262	-22627.9008	-4116177.36
-149140.055536	50.095032	-1.2071676000E-05	-572.49672	1672177.44
024363.572054	11.395124	.000069550016	2733.76376	2271409.92
-3717.71063072	12.472504	0	0	0
-04114.5446491	31.1360992	-.000024608196	-6217.0424	23734.9952
-361013.397391	56.709432	.000066571624	-9200.616	1763007.04
213029.200601	12.472504	0	0	0
166504.003264	34.705776	-.000000050100	-20092.0232	-7042409.6
136535.102059	32.0095072	.0003125440	-21050.072	-9412744.0
50544.6435647	63.224032	-.00039459304	-45940.608	-16417179.2
044161.136090	06.474912	-.0036015072	-90479	-39617040.0
-229457.536972	51.002104	.00022566404	3300.2032	3017565.20
105501.17903	30.610512	.000010425002	-4353.452	630021.60
30705.1226616	31.6511232	-.000060705152	-7030.7744	-657139.04
214445.050405	9.604372	.00029773344	4427.5000	2050327.36
32104.6956292	29.47620	.00066230620	-6264.7032	-2102250.0
-794.96	31.740192	0	0	0
-297115.020612	37.5664624	.0001006442	-407.195240	050933.36
-1632491.4404	136.540632	0	0	0
-1471365.00672	146.423264	.00103290940	-37420.4400	-12025234.4
-40329.1736109	22.9040520	.0003199714	3400.71336	5429150.4
102390.354976	31.5507072	-.00006074312	-7172.2120	-392011.512
691553.916429	30.02752	.00074033700	-37192.4120	-24657567.2
750476.029092	66.613464	.0002391156	-43001.792	-20691553.6
530335.412099	59.37100	-.000015466156	-1052.10064	2403959.04
-09326.0112904	204.334000	.000136402504	-31427.2792	-2969301.12
204943.717066	62.76	-.0003023906	-26215.6000	-5946719.2
36016.0669367	03.592136	-.00047406012	-20200.9112	-4749676.0
90275.7402103	56.166016	-.0003527112	-19233.4296	-2344797.20
54534.0209901	05.5620	-.00060937060	-32361.5664	-1612011.52
474009.050311	92.010712	-.00002674622	-42593.12	-10530659.2
916056.300099	40.906776	.0002015032	-16105.3056	-3220090.00

3. Chemical Species Symbols

Al  
AlH  
AlOH  
Al<sub>2</sub>O  
Al<sup>+</sup>  
Ar  
CO  
CO<sub>2</sub>  
H  
OH  
H<sub>2</sub>  
H<sub>2</sub>O  
AlO  
AlO<sub>2</sub>  
HO  
H<sub>2</sub>  
O  
O<sub>2</sub>  
Al(l)  
AlN  
Al<sub>2</sub>O<sub>3</sub>(l)  
Al<sub>2</sub>O<sub>3</sub>(s)  
C(s)  
CH<sub>4</sub>  
CH<sub>3</sub>  
C<sub>2</sub>H<sub>6</sub>  
C<sub>2</sub>H<sub>4</sub>  
Al<sub>2</sub>C<sub>3</sub>  
HCH  
HNC  
HCO  
CH<sub>3</sub>  
C<sub>2</sub>H<sub>2</sub>  
C<sub>2</sub>H<sub>4</sub>  
C<sub>2</sub>H<sub>6</sub>

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