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Characterization of Rocket Propellant Combustion Products

Chemical Characterization and Computer Modeling of the Exhaust Products from Four Propellant Formulations

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CHARACTERIZATION OF ROCKET PROPELLANT COMBUSTION PRODUCTS

SUBTITLE: CHEMICAL CHARACTERIZATION AND COMPUTER MODELING OF THE EXHAUST PRODUCTS FROM FOUR PROPELLANT FORMULATIONS

Final Report

DOE Interagency Agreement No. 1016-1844-A1
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December 9, 1991

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The objective of this work was the determination of the chemical composition of exhaust products from the firing of scaled down rocket motors at the Army Signature Characterization Facility at Redstone Arsenal, and the comparison of those results with component levels predicted by a selected computer model. Both real time and off-line sampling and analysis approaches were employed. Four types of propellant compositions were evaluated. CO levels ranged from 85 - 350 ppm, while particle concentrations ranged from 30 - 100 mg/m^3. All of the airborne particles were in the inhalable range. For two of the propellants, airborne lead was greater than 10 mg/m^3. For the predominantly perchlorate formulation, hydrogen chloride (HCl) levels were greater than 100 ppm. Particulate PAH levels were about a factor of 10 lower than that in outside ambient air particulate matter. The computer model predicted mole fractions for CO were typically 20 - 35%, except for the predominantly inorganic formulation. The model correctly predicted only minor amounts of ammonia and essentially no hydrogen cyanide. The accuracy of the predicted CO/CO_2 ratios was low for all but one of the formulations. A modification of the model accomplished by mathematically accounting for mixing of hot exhaust gases with ambient air brought the predicted CO/CO_2 ratio into greater agreement with that which was observed experimentally.

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Roger A Jenkins December 20, 1991

PI Signature Date

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EXECUTIVE SUMMARY

The overall objective of the work described in this report is four-fold: to a) develop a standardized and experimentally validated approach to the sampling and chemical and physical characterization of the exhaust products of scaled-down rocket launch motors fired under experimentally controlled conditions at the Army's Signature Characterization Facility (ASCF) at Redstone Arsenal in Huntsville, Alabama; b) determine the composition of the exhaust products; c) assess the accuracy of a selected existing computer model for predicting the composition of major and minor chemical species; d) recommend alterations to both the sampling and analysis strategy and the computer model in order to achieve greater congruence between chemical measurements and computer prediction.

Analytical validation studies were conducted in small chambers at the Oak Ridge National Laboratory (ORNL), while the actual firings were conducted at Redstone Arsenal. Real time determination of selected species was performed by a variety of techniques, including non-dispersive infrared spectrometry, chemiluminescence, electrochemical monitoring, and optical scattering. Samples for analyses of trace constituents were collected from individual firings in the ASCF, and returned to ORNL for analysis, usually by gas chromatography/mass spectrometry. Four types of propellants were examined: a double base, a double base with 8% potassium perchlorate, one propellant which was predominantly ammonium perchlorate, and a minimum signature reduced smoke propellant, which was about two-thirds octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (HMX). Small, 2x2 motors, containing 25 - 75 g of propellant, produced significant quantities of carbon monoxide (CO) and particles when fired into the 20 m^3 chamber. CO levels ranged from 85 - 350 ppm. This is equivalent to reaching 2500 - 7500 ppm if a full scale motor was fired in a similarly sized enclosed environment. Particle concentrations ranged from 30 - 100 mg/m^3. All of the airborne particles were in the inhalable range. For two of the propellants (the double base and the minimum signature), airborne lead was greater than 10 mg/m^3. No ammonia or hydrogen cyanide was detected above 1 ppm. For the predominantly perchlorate formulation, hydrogen chloride (HCl) levels were greater than 100 ppm in the ASCF chamber. Because of the relatively high background levels observed, trace organic vapor phase constituents were difficult to accurately quantify. While a wide variety of trace constituents were observed, only a few were present at levels greater than a few ppbv. Compounds present at levels greater than 10 $\mu g/m^3$ included benzene, methyl crotonate, toluene, and cyanobenzene. A number of PAHs and nitrofluorene were observed in the airborne particulate matter. However, the levels were about a factor of 10 lower than that in outside ambient air particulate matter at a military installation.

Computer modeling was performed with the NASA-Lewis CET-86 version. This approach obtains estimates of equilibrium concentrations by minimizing free energy. Mole fractions of major and minor species were estimated for a range of exit/throat area ratios. The predicted mole fractions for CO were typically 20 - 35%, except for the predominantly inorganic formulation. The model correctly predicted only minor amounts of ammonia

and essentially no hydrogen cyanide. Predicted mole fractions did not vary a great deal with such input parameters as exit/throat area ratios or small changes in the heats of formation of the various compositions. The accuracy of the predicted CO/CO_2 ratios was low for all but one of the formulations. In general, if the model were to be used in its present state for health risk assessments, it would be likely to over-estimate exposure to CO.

Probably the greatest limitation of the model is its inability to account for reactions after hot exhaust gases leave the rocket motor nozzle. For example, the model predicted no significant quantities of NO would be produced, yet such was measured at ppm levels on every burn. A modification of the model accomplished by mathematically accounting for mixing of hot exhaust gases with ambient air brought the predicted CO/CO_2 ratio into greater agreement with that which was observed experimentally. It seems likely that with the appropriate modifications to account for the roles of kinetically governed processes and the afterburning of exhaust gases, the model could make a more accurate prediction of the amounts of the major products. However, it seems unlikely for the system to be modifiable to the extent to which accurate predictions of toxic or carcinogenic species present at the ppbv level could be made.

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I. OBJECTIVES

The overall objective of the work described in this report is four-fold: to a) develop a standardized and experimentally validated approach to the sampling and chemical and physical characterization of the exhaust products of scaled-down rocket launch motors fired under experimentally controlled conditions at the Army's Signature Characterization Facility (ASCF) at Redstone Arsenal in Huntsville, Alabama; b) determine the composition of the exhaust products; c) assess the accuracy of a selected existing computer model for predicting the composition of major and minor chemical species; d) recommend alterations to both the sampling and analysis strategy and the computer model in order to achieve greater congruence between chemical measurements and computer prediction.

II. BACKGROUND

Upon initiation of the Army's Health Hazard Assessment Program in 1983, the lack of information on the potential health hazards from weapons combustion products, to include rockets and missiles, became evident. Research to elucidate significant health effects of rocket and missile combustion products has been limited. Experiences with weapons systems such as ROLAND, VIPER, HELLFIRE, STINGER, and MLRS have resulted in the development of specific medical issues by the U.S. Army. Presumably, these issues will be addressed, in order to enhance the effectiveness of soldiers using such weapons. Requisite to addressing these issues is defining the chemical and physical nature of the combustion products.

Evaluation of rocket exhaust toxicity from Army missile and rocket systems has been directed towards a limited number of combustion products. Chemical species such as carbon monoxide, carbon dioxide, nitrogen, oxides of nitrogen, hydrogen chloride, sulfur dioxide, ammonia, lead, and copper are among those frequently evaluated. A USAMRDC study[1] has demonstrated more than one hundred chemical species in the combustion products of selected propellants. Many of the species represent potential health hazards even though the majority of those identified were at low levels. During the study, data were obtained for the Multiple Launch Rocket System's (MLRS) propellant by computer prediction and laboratory analyses. The combustion product was generated by burning the propellant in a small test motor. When the exhaust plume was vented into a chamber with an inert atmosphere, good quantitative data was obtained for twelve chemical species, and was in excellent agreement with theoretically computed values. In excess of fifty trace gas species also were qualitatively identified.

Various investigators have examined propellant and related combustion products generated in a variety of ways to include directly from a weapon or other equipment system[1-5], burning in a calorimeter or bomb[6-9], personal and general area sampling in indoor firing ranges[10,11], and detonation or combustion in chambers or microcombustors[2,14-17]. The methods of sampling and characterization also have been varied. Sampling has been done under atmospheric[1,2,4,5,12,16], and less than atmospheric[1-3,8,9,13-15] conditions which provide a basis for comparing the relation between variables, such as, pressure and available oxygen, on the composition of the combustion product. Sampling methods have been either direct and continuous, e.g., the method used by Goshgarian[13,14] where the exhaust products of solid propellants were introduced directly into a mass spectrometer for analysis immediately following combustion, or by collection in a container or on a medium for subsequent analysis. The latter has involved cryogenic trapping, evacuated glass or stainless steel cylinders, and sorbent cartridges, filters, and condensation trains. Analytical methods to detect organics, gases, metals, and particulates have included gas chromatography (GC), gas chromatography-mass spectroscopy (GC-MS), titration, optical and infrared spectroscopy, scanning electron microscopy (SEM), x-ray emission and diffraction, and particle size analysis. Because of limitations with each sampling and analytical technique, several techniques must be employed simultaneously to optimize qualitative and quantitative characterization.

Computer models have been used to predict propellant ballistic properties to include the identity of the major chemical species contained in the combustion products[1,3,5,17-19]. When compared with laboratory derived empirical data, the models tend better to predict the major species than the minor ones both qualitatively and quantitatively[1,5,19]. The models predict the chemical species that occur at the nozzle of the rocket as the exhaust exits; however, afterburning changes the chemical content of the combustion product. Afterburning and incomplete combustion effects are not predicted by the models.

The approach taken in this study was to carefully validate real time analytical methods in chamber studies at Oak Ridge National Laboratory (ORNL) for as many of the major constituents as practical. The instrumentation for real time monitoring would then be transported to the ASCF for the firing of the scaled-down test motors. Vapor and particle phase samples for determination of trace organics and metal species would be returned for analysis. The Army Signature Characterization Facility (ASCF) has been used to determine the concentrations of major toxic species in propellant exhaust, e.g., carbon monoxide, carbon dioxide, hydrogen chloride, lead, aluminum oxide, and other nuisance particles[20]. The facility is a 19.6 m^3 walk-in, climatic chamber with temperature limits of -40° to 140°F and humidity control in the range of 20 to 100% relative humidity (RH). Typical operating parameters are 70°F and 60% RH. Designed as a smoke measurement facility, the ASCF has been adapted for the measurement of rocket motor signature and exhaust constituents. The facility serves as a large gas cell in which the exhausts of standard 2 x 2 motors can be measured by infrared spectroscopy (Fourier Transform Infrared Spectroscopy, FTIS). Ports in the ASCF allow sampling and measurement by other methods, e.g., air sampling pumps and direct reading instruments.

The results of the characterization studies were then to be compared with values predicted using the most recent version of a computer model developed by the Lewis Research Center of the National Aeronautics and Space Administration (NASA-Lewis). The model was then to be refined to the extent of available resources, in order to improve the predictive capability of the system.

Results of these studies are described in two parts. In Part 1, results of the chemical and physical characterization studies are described and discussed. In Part 2, results of the computer modeling work are described. Comparisons with characterization data are performed, and recommendations for model improvement are made.

PART 1: CHEMICAL CHARACTERIZATIONSTUDIES

EXPERIMENTAL

The sampling and analysis methods used in this study have been described in detail in a previous report[21], and are summarized in Table 1. An assortment of real-time analytical instrumentation was employed. However, resources were not available for the use of on-line mass spectrometric measurement, as such would have required periodic transport to the ASCF. Essentially, the approach taken was to first validate candidate analytical methods in small chambers (0.4 and 1.4 m^3) at ORNL. Analytical measurements using real time instrumentation were made of target species in the presence of well defined quantities of other species. The extent to which these materials altered the response to the target species was noted, and corrections made when appropriate. For species which could not be determined in real time (usually trace organic vapor phase and particle phase species), samples would be taken at the actual burns to be conducted at the ASCF, and returned to ORNL for detailed chemical analysis. Following method validation for the propellant composition of interest, the sampling and analysis instrumentation was transported to the ASCF at Redstone Arsenal, and deployed for monitoring and sampling. Typically, between 2 and 3 firings of a test motor could be conducted during each 8-hour shift. Burns of the various propellant formulations took place between August, 1987 and December, 1989.

RESULTS AND DISCUSSION

The compositions of the various propellant formulations tested in this project are listed in Appendix A. Briefly, Composition D was a double-base propellant, comprised of approximately 50% nitrocellulose and about 40% nitroglycerine. Composition H was also a double base system, with approximately 8% by weight of potassium perchlorate added. Composition L was a formulation comprised of nearly 75% ammonium perchlorate, with the remainder being polyvinylchloride plastic and di (2-ethylhexyl) adipate. Composition Q was a minimum signature propellant, comprised of 66% HMX, and about 11% each of nitroglycerine and butane triol trinitrate. (A fifth motor, referred to as Composition X was fired only one time, and no modeling studies were applied to it.) (Note that the linkage between the propellant and the weapon systems for which they may be used is considered CLASSIFIED information. Those having need of this information should contact the COR listed on the title page of this document.) All of the propellants contained small amounts of metals. The motor size tested varied between ca. 24 - 75 g. This compares to a typical launch motor weight on an anti-tank weapon system of ca. 560 g.

Sampling of the exhausts was not without its difficulties. For example, for the first run of Composition D, the high volume particulate collector was placed inside the ASCF chamber. However, the shock wave from the firing was sufficient to blow the filter media out of the holder. Thus, for subsequent runs, the sampler was placed outside the chamber and

TABLE 1
Summary of Sampling and Analysis Strategy for Rocket Exhaust Constituents at ASCF

Component	Sampling and Analysis Method
Carbon Monoxide	Real Time, non-dispersive infrared analyzer
Carbon Dioxide	Real time, non-dispersive infrared analyzer
Oxides of Nitrogen	Real time, chemiluminescence analyzer
Hydrogen Cyanide	Real time, electrochemical analyzer
Ammonia	Real time, electrochemical analyzer
Hydrogen Chloride	Real time, ion selective electrode
Total Suspended Particulate Matter	Real Time: forward scattering infrared photometer
	Off line: two-stage high volume filter, gravimetric analysis
Metals	Low volume collection on membrane filter, followed by inductively coupled plasma or atomic absorption analysis.
Particle Size Distribution	Cascade impaction, optical comparison of stages
Trace Vapor Phase Organics	Collection on multi-sorbent traps, followed by thermal desorption gas chromatography/mass spectrometric analysis.
Trace Particle Phase Organics	Collection on two-stage, high volume filter, analysis by high performance liquid chromatography and/or gas chromatography/mass spectrometry.

connected to it with the flexible plastic pipe. Also, on a latter run with "D,"the force of the shock wave buckled the main chamber access door on the ASCF. For the final firing of "D,"the nozzle was changed to force the propellant to burn over a longer period of time. This resulted in a considerable alteration in the exhaust composition (see Table 2).

Major Constituents

The observed exhaust major constituent concentrations in the ASCF are reported in Tables 2 - 5, along with various physical characteristics of the motors. The data is summarized in Table 6.

It is important to note that for those constituents determined in real time (ie, the gases), the concentrations listed represent peak concentrations. For gases, maxima were typically achieved within 30 seconds of the firing of the rocket motors. Presumably, maxima were achieved as the chamber contents were mixed by the fan mounted inside the chamber. Such was not always the case for the particulate phase species. For example, in Figures 1 and 2 are compared the time courses for some of the major exhaust products for firings of Composition D and H motors, from about 30 seconds following the firing onward. For Composition D, immediately after following the achievement of maximum concentrations, the constituent levels slowly decreased. While the same happened for Composition H vapor phase species, the particles were very slow to reach a maximum. Although particle

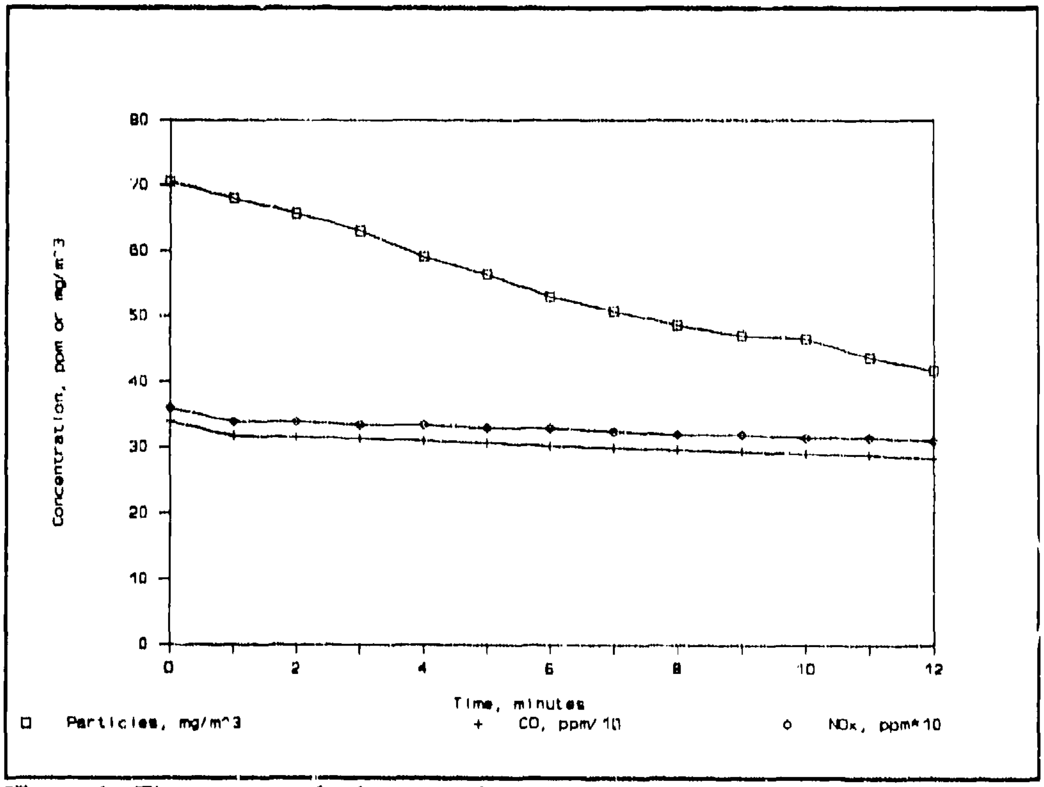

Figure 1. Time course of exhaust products post firing. Composition D.

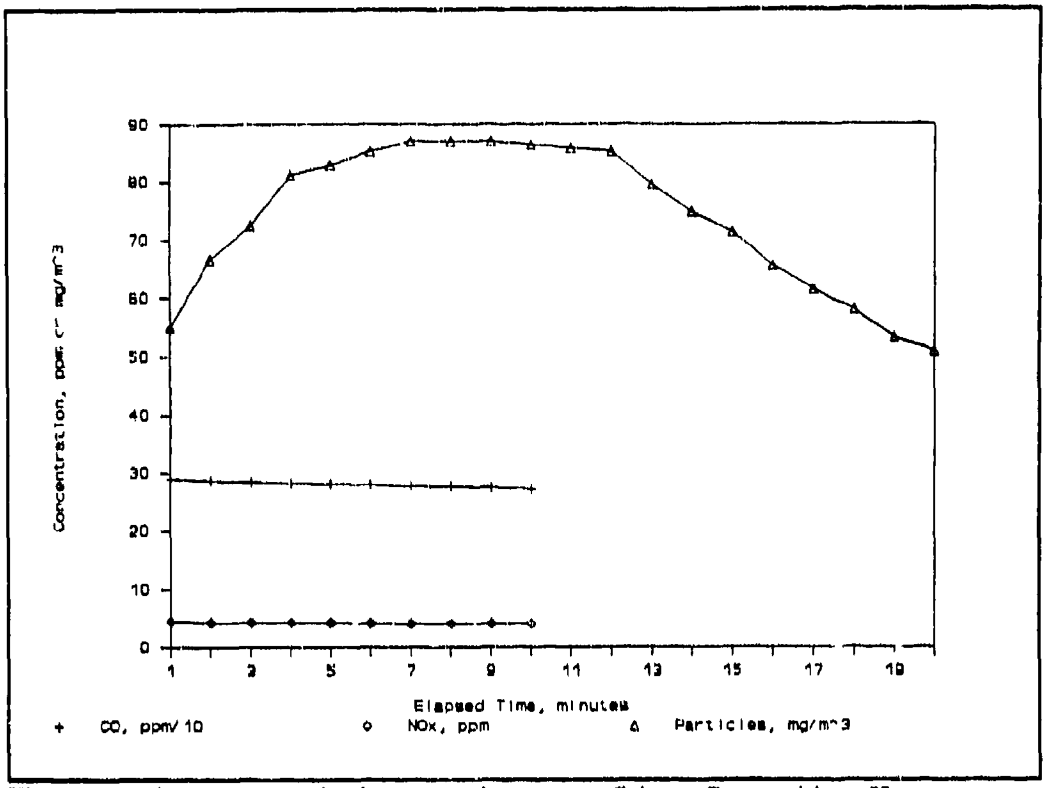

Figure 2. Time course of exhaust products post firing. Composition H.

size differences between the two products were minimal (see below), it was speculated that the action of the fans could have stirred up larger agglomerates which settled immediately after firing, which eventually broke up to form smaller primary particles. Concentration reductions seemed most likely due to leaking of the chamber contents through door seals, bulkheads, etc. Particle concentrations decreased somewhat more rapidly than those of vapor phase constituents, probably due to settling.

No attempt was made to determine the concentrations of methane, hydrogen gas, or water vapor. For the former two species, quantitative measurements would be very difficult without the use of an on-line mass spectrometer, and such was not available for this work. Water vapor is one of the major components of the motor exhaust. The mole fraction predicted by the NASA-Lewis computer program typically is in the range of 20% (see below). However, the difficulty of making accurate determinations of water vapor concentration in a large chamber is considerable. For example, the maximum amount of hydrogen in any of the formulations listed in Tables A-1 - A-4 is sufficient to produce only 15 g of H_2O in the 20 m^3 ASCF chamber. This is comparable to increasing the concentration by at most 0.75 g/m^3, to a concentration of ca. 11 g/m^3 at 60% relative humidity at 21° C. The addition of this amount of water vapor would increase the RH by 4%, as long as no change in the temperature occurred. Given that such small changes would be difficult to measure accurately, and that water vapor poses no health hazard,

TABLE 2

SUMMARY OF CHARACTERIZATION DATA
COMPOSITION D
MAJOR CONSTITUENTS

RUN NUMBER	1	2	3	4	5	6[d]
DATE	8-25-87	8-25-87	8-26-87	8-26-87	6-23-88	6-23-88
QUANTITY OF PROPELLANT, g	75	71	75	75	67	NR
EXIT DIAMETER, inches [a]	1.0	1.0	1.0	1.0	1.0	1.0
THROAT DIAMETER, inches	0.55	0.707	0.50	0.50	0.50	NR
ASCF CHAMBER TEMPERATURE, °F	71	78	71	71	68	71
ASCF RELATIVE HUMIDITY, %	76	60	60	60	69	87
INTERNAL PRESSURE OF MOTOR, psia	2200	2500	3000	2500	2500	2500
CARBON MONOXIDE[b], ppm	292	367	340	325	282	139
CARBON DIOXIDE[b,c], ppm	2200	2500	3000	2500	1245	1505
NITRIC OXIDE[b], ppm	4.2	3.0	3.6	3.5	2.2	43.0
NITROGEN DIOXIDE[b], ppm	ND	ND	ND	ND	ND	ND
HYDROGEN CYANIDE[b], ppm	ND	ND	ND	ND	ND	ND
AMMONIA, ppm	ND	0.2	ND	ND	ND	ND
TOTAL SUSPENDED PARTICULATE MATTER, mg/m^3	71	63	71	70	67	NR
LEAD mg/m^3	18	35	73	40	36.9	41.8
COPPER mg/m^3	2.0	3.8	9 1	4.4	4.0	4.8
ALUMINUM (as AL_2O_3) mg/m^3	ND	ND	ND	ND	ND	ND
CHROMIUM mg/m^3	ND	ND	ND	ND	ND	ND
ZIRCONIUM OXIDE mg/m^3	ND	ND	ND	ND	ND	ND

[a] Nominal exit diameter was 1.0 inches. However, this was an estimate only. Actual diameters could have varied between 0.75 and 1.25 inches.
[b] Maximum observed concentrations.
[c] Determined in Runs 1-4 using Draeger Tubes, Runs 5 and 6 using NDIR analyzer.
[d] Special nozzle used which increased burn time. See text. Data may not be representative.
NR: Not Recorded
ND: Not Detected

TABLE 3

SUMMARY OF CHARACTERIZATION DATA
COMPOSITION H
MAJOR CONSTITUENTS

RUN NUMBER	1	2	3	4
DATE	6-22-88	6-22-88	6-22-88	6-23-88
QUANTITY OF PROPELLANT, g	25	25	24	24
EXIT DIAMETER, inches [a]	1	1	1	1
THROAT DIAMETER, inches	0.261	0.261	0.261	0.261
ASCF CHAMBER TEMPERATURE, °F	70	70	70	72
ASCF RELATIVE HUMIDITY, %	NR	68	57	63
INTERNAL PRESSURE OF MOTOR, psia	5000	5000	5000	5000
CARBON MONOXIDE[b], ppm	290	c	300	298
CARBON DIOXIDE[b], ppm	250	c	270	290
NITRIC OXIDE[b], ppm	4.5	c	1.7	5.0
NITROGEN DIOXIDE[b], ppm	ND	c	ND	ND
HYDROGEN CYANIDE[b], ppm	ND	c	ND	ND
HYDROGEN CHLORIDE, ppm	<1		<1	1
AMMONIA[b], ppm	ND	c	ND	ND
TOTAL SUSPENDED PARTICULATE MATTER, mg/m^3	87	c	73	176
LEAD mg/m^3	0.771	c	0.618	0.486
COPPER mg/m^3	0.726	c	0.807	0.500
ALUMINUM (as AL_2O_3) mg/m^3	ND	c	ND	ND
CHROMIUM mg/m^3	ND	c	ND	ND
ZIRCONIUM OXIDE mg/m^3	ND	c	ND	ND
MOLYBDENUM, mg/m^3	1.41	c	0.309	0.088
MAGNESIUM, mg/m^3	0.261	c	0.224	0.250
TIN, mg/m^3	0.348	c	0.397	0.177

a Nominal exit diameter was 1.0 inches. However, this was an estimate only. Actual diameters could have varied between 0.75 and 1.25 inches.
b Maximum observed concentrations.
c Sample Acquisition failure.
NR: Not Recorded
ND: Not Detected

Table 4

SUMMARY OF CHARACTERIZATION DATA
COMPOSITION L
MAJOR CONSTITUENTS

RUN NUMBER	1	2	3	4
Date	1-18-89	1-18-89	1-19-89	1-19-89
Quantity of Propellant, g	24	24	24	24
Exit Diameter, inches [a]	1.0	1.0	1.0	1.0
Throat Diameter, inches	0.28	0.28	0.28	0.28
ASCF Chamber Temperature, °F	69	70	71	70
ASCF Relative Humidity, %	NR	68	49	48
Internal Pressure of Motor, psia	2500	2500	2500	2500
Carbon Monoxide[b], ppm	298	337	371	371
Carbon Dioxide[b], ppm	164	137	164	150
Nitric Oxide[b], ppm	1.5	0.5	0.5	0.5
Nitrogen Dioxide[b], ppm	ND	ND	ND	ND
Hydrogen Cyanide[b], ppm	ND	ND	ND	ND
Ammonia[b], ppm	ND	ND	ND	ND
Hydrogen Chloride, ppm	112	112	108	122
Total Suspended Particulate Matter, mg/m^3	50	33	38	51
Lead mg/m^3	2.73	2.71	1.52	1.50
Copper mg/m^3	5.74	4.43	3.98	3.80
Aluminum (as Al_2O_3) mg/m^3	4.33	3.62	3.35	3.14
Chromium mg/m^3	0.64	0.52	0.52	0.46
Zirconium Oxide mg/m^3	ND	ND	ND	ND
Cadmium, mg/m^3	0.15	0.13	0.12	0.11

a Nominal exit diameter was 1.0 inches. However, this was an estimate only. Actual diameters could have varied between 0.75 and 1.25 inches.
b Maximum observed concentrations.
NR: Not Recorded
ND: Not Detected

Table 5

SUMMARY OF CHARACTERIZATION DATA
COMPOSITION Q
MAJOR CONSTITUENTS

RUN NUMBER	1	2	3
Date	12-1-89	12-5-89	12-5-89
Quantity of Propellant, g	65	64	60
Exit Diameter, inches [a]	1.125	1.125	1.125
Throat Diameter, inches	0.188	0.190	0.197
ASCF Chamber Temperature, °F	66	63	64
ASCF Relative Humidity, %	34	46	40
Internal Pressure of Motor, psia	1580	1480	1100
Carbon Monoxide[b], ppm	84	84	93
Carbon Dioxide[b], ppm	1350	1324	1194
Nitric Oxide[b], ppm	2	1	1
Nitrogen Dioxide[b], ppm	ND	ND	ND
Hydrogen Cyanide[b], ppm	ND	ND	ND
Ammonia[b], ppm	ND	ND	ND
Total Suspended Particulate Matter, mg/m^3	31	28	29
Lead mg/m^3	18.6	1.5	14.1
Copper mg/m^3	0.002	0.00	0.01
Aluminum (as AL_2O_3) mg/m^3	ND	ND	ND
Chromium mg/m^3	0.0	0.02	0.02
Zirconium Oxide mg/m^3	<0.1	<0.1	0.06
Iron, mg/m^3	0.33	0.06	0.06

a Nominal exit diameter was 1.0 inches. However, this was an estimate only. Actual diameters could have varied between 0.75 and 1.25 inches.
b Maximum observed concentrations.
NR: Not Recorded
ND: Not Detected

TABLE 6

MEAN CONCENTRATIONS ACHIEVED IN ASCF CHAMBER

Constituent	Propellant Formulations (approximate motor size)				
	D (75 g)	H (25 g)	L (22 g)	Q (63 g)	X (25 g)
CO, ppm	330	295	344	85	195
CO_2, ppm	1375	270	154	1250	561
NH_3, ppm	BMDL	BMDL	BMDL	BMDL	BMDL
NO, ppm	3.5	4	0.75	1.3	5.0
NO_2, ppm	BMDL	BMDL	BMDL	BMDL	BMDL
HCN, ppm	BMDL	BMDL	BMDL	BMDL	BMDL
HCl, ppm	BMDL	<1	114	BMDL	BMDL
Particles, mg/m^3	70	100	43	30	45
Pb, mg/m^3	40	0.6	2	16	0.18
Cu, mg/m^3	4	0.7	4	0.01	0.45
Al_2O_3, mg/m^3	BMDL	BMDL	3.5	BMDL	BMDL
Cr, mg/m^3	BMDL	BMDL	0.5	0.01	1.3
Cd, mg/m^3	BMDL	BMDL	0.13	BMDL	BMDL
Sn, mg/m^3	BMDL	0.3	BMDL	BMDL	BMDL

* BMDL: Below method detection limit.

it was decided that determination of water vapor would be omitted from the measurements.

A determination of the carbon balance for the chamber indicates that the analytical measurements account for approximately 60% of the carbon in the formulation. For example, using the data in Table A-1 for Composition D, there are ca. 2.06 moles of carbon in the motor. Data from Run 5 of the "D" test indicates ca. 1.2 moles of C tied up as the oxides of carbon (CO and CO_2). The analysis of the vapor and particle phase organic constituents (see below) indicates that only a very tiny amount of C is tied up in the trace species. And even if all the non-metal material collected as particulates was pure carbon, such would only add ca. 26 mg/m^3 of carbon, or about 0.043 moles. Thus, it would appear that a significant fraction of the carbon present in the motor itself (ca. 33%) is present in some form which is not amenable to conventional analyses. Without confirmatory data, the composition of such material would be highly speculative.

All of the formulations, despite the relatively small quantities of propellant fired in the chamber (ca. 1/7 to 1/20 of a typical size launch motor) produced substantial concentrations of carbon monoxide, ranging from a low of about 300 ppm/100 g of propellant for Composition Q, to a high of nearly 1400 ppm/100 g for Composition L. The amounts of carbon dioxide produced varied considerably, from more than a factor of 10 greater than the CO produced, to only about half the amount of CO produced. Only very small quantities of nitric oxide were produced, and no measurable amounts of nitrogen dioxide were produced. The latter is not surprising, since the production of NO_2 is dependent on the square of the NO concentration[22]. If the concentration of NO is low, significant amounts of the dioxide will not be produced in the first 10 minutes following the firing of the motor (the duration of time for which the ASCF was sampled for the oxides of nitrogen). Essentially, no ammonia or hydrogen cyanide was found at levels greater than 1 ppm. In the two formulations which contained perchlorates, measurable levels of hydrogen chloride were found. However, the observed levels were not proportionate to amount of perchlorate present. For example, while Composition L had about 8x more perchlorate in the formulation than Composition H, the levels observed in the chamber were about 100x larger. There were a number of metals found in the airborne particles resulting from motor firings. Copper, aluminum (as the oxide), lead, tin, chromium, and cadmium were all found in measureable amounts. Probably the lead and cadmium are of the greatest concern from a health risk standpoint. For both Compositions D and Q, lead was found to be present in the diluted exhaust at levels greater than 10 mg/m^3.

In Table 7 are listed the particle size distributions of the exhaust products for the formulations studied. The mass median aerodynamic diameters (MMAD) were all less than 2 μm, indicating that the particles remaining airborne long enough to be collected by the sampling method were capable of being inhaled. Although Composition D had a measurably bimodal distribution, the higher of the two MMADs was still less than 5 μm. Particles from Composition L had a somewhat smaller MMAD than of the other formulations, but the breadth of the distribution was larger.

TABLE 7

Particle Size Distribution
Rocket Exhaust Particulate Matter
Mean Values

Mass Median Aerodynamic Diameter (MMAD) and Geometric Standard Deviation (σ_g)

Composition	MMAD (μm)	σ_g
D[a]	1.46	1.86
H	1.44	1.77
L	0.807	2.14
Q	0.96	2.4

[a] Composition D had a definite bimodal distribution: large particles had a MMAD of 3.6 microns, with $\sigma_g = 1.8$; small particles had a MMAD of 0.47 microns, with $\sigma_g = 1.7$.

Trace Constituents

Trace organic vapor phase constituents present in the exhaust atmospheres were determined by collection of samples on multi-sorbent traps, followed by analysis by thermal desorption GC/MS. Because of the sensitivity of the method, collection of sufficient sample was not difficult. However, the background levels of vapors in the chamber were very high, and as a result, made it very difficult to discern quantities of vapors arising from the firing of the rocket motor. Despite the fact that the chamber was flushed with clean air between most firings, background levels of collected constituents on chamber blanks were substantial (see Table 8). This suggests that there may be significant off-gassing of volatiles from materials adsorbed on the surfaces inside the chamber. Accurate quantitative determination of the constituents identified was exceedingly difficult, because it required determining the difference between two large values. Also, the largest peak in many of the samples was determined to be a mixture of hydrocarbons that were not resolved, even by high-resolution chromatography. These may be unburned, volatilized waxes used in the manufacture of the test motors. In Appendix B, in Tables B-1 through B-4, are listed the various trace organic vapor phase components identified and quantified in the exhaust. The data is summarized in Tables 9 - 12. In this case, mean quantities were reported only if the compound was observed in two or more of the traps analyzed from the firing of a specific composition and if the compound was present at a level 50% greater than the highest level reported for any blank collected during the series of firings. Several comments are in order. First, as stated above, it was very difficult to obtain a truly "clean" chamber atmosphere into which to fire the motors.

Table 8

CONCENTRATION OF SELECTED CONSTITUENTS IN CHAMBER BLANKS

	Concentration $\mu g/m^3$		Concentration $\mu g/m^3$
		C_3-cyclopentane	52.4
Methylene chloride	11.9	C_{12}-cyclohexasiloxane	8.2
Methyl crotonate	2.1	C_{12}-cyclohexasiloxane	4.4
C_6-cyclotrisiloxane	23.9	C_3-cyclopentane	7.4
C_8-cyclotetrasiloxane	7.5	Diethylphthalate	19.1
C_3-cyclopentane	25.4	Pentadecane	2.1
Terpinene	8.8	Nonadecane	2.6
C_{10}-cyclopentasiloxane	12.9	Trimethylcyclobutanone	3.5
Naphthalene	8.8		

Originally, it was believed that the siloxane compounds may have resulted from contamination of the multi-sorbent traps with a soap bubble solution which was used in measuring the sample flow rates in some of the earlier studies. (This potential for contamination has been confirmed by subsequent experiments in the laboratory). However, the siloxanes were also present in the blanks which were acquired in later experiments, in which only instrumental calibration of the flow rates were made. Thus, the siloxanes may be off-gassed byproducts of the detergents used to clean the chamber prior to the motor firings, or they may be true products of the propellant combustion. Significant amounts of siloxane have been seen in the vapor phases of several of the exhausts from various motors. In general, there appeared to be a greater variety of trace organics present in the vapor phase of the composition D and H exhausts. The fact that Composition L is predominantly inorganic probably contributes to this observation.

Table 13 summarizes the maximum observed concentrations of non-siloxane compounds found in the ASCF atmospheres for those constituents with levels greater than 10 $\mu g/m^3$ (ca. 3 ppbv for benzene). For example, the average concentration for benzene was 17.6

$\mu g/m^3$ or 5.4 ppb. Overall, the concentrations of these species were several orders of magnitude below the levels at which they are regulated for workplace exposures. One may conclude table 9

TABLE 9
ESTIMATED CONCENTRATION OF TRACE VAPOR PHASE CONSTITUENTS
COMPOSITION D

CONSTITUENT	APPROXIMATE CONCENTRATION*, $\mu g/m^3$
Trichloroethane	0.4
Benzene	13.5
Trichloroethylene	2.0
Methyl crotonate	15.3
Toluene	10.5
C_6-cyclotrisiloxane	11
C_2-benzene	5.7
Phenylacetylene	2.7
Styrene	4.7
C_3-benzene	2.7
C_3-benzene	3.9
Decane	1.5
Decane	0.9
Terpinene	0.7
C_8-cyclotetrasiloxane	15
Teripene	1.1
Undecane	0.8
Naphthalene	6.1
C_3-cyclopentane	1.3
Dodecane	0.7
C_{12}-cyclohexasiloxane	17.8
Hexadecane	1.1

* Estimated by determination of mean value for at least 2 of traps analyzed, which must be at least 50% greater than the highest blank level observed. Levels have been corrected for blanks.

TABLE 10
ESTIMATED CONCENTRATION OF TRACE VAPOR PHASE CONSTITUENTS
COMPOSITION H

CONSTITUENT	APPROXIMATE MEAN CONCENTRATION[a], $\mu g/m^3$
Trichlorofluoromethane	9.8
Trichloroethane	0.4
Benzene	17.6
Methylcrotonate	7.0
Toluene	2.2
Phenylacetylene	2.4
C_2-benzene	0.7
Heptene	8.4
Cyanobenzene	18.0
C_3-benzene	1.4
C_3-cyclopentane	16.1
C_{14}-cycloheptasiloxane	2.2

[a] Estimated by determination of mean value for at least 2 of traps analyzed, which must be at least 50% greater than the highest blank level observed. Levels have been corrected for blanks.

TABLE 11
ESTIMATED CONCENTRATION OF TRACE VAPOR PHASE CONSTITUENTS
COMPOSITION L

CONSTITUENT	APPROXIMATE MEAN CONCENTRATION[a], $\mu g/m^3$
Octamethyl-cyclotetrasiloxane	3.5
Octamethy-cyclotetrasiloxane	2.6

[a] Estimated by determination of mean value for at least 2 of traps analyzed, which must be at least 50% greater than the highest blank level observed. Levels have been corrected for blanks.

TABLE 12
ESTIMATED CONCENTRATION OF TRACE VAPOR PHASE CONSTITUENTS
COMPOSITION Q

CONSTITUENT	APPROXIMATE MEAN CONCENTRATION[a], $\mu g/m^3$
trichlorofluromethane	0.6
hexamethyl cyclotrisiloxane	0.2
trimethyl-cyclobutanane	23.5
octamethyl-cyclotetrasiloxane	0.3
phthalate	8.5

[a] Estimated by determination of mean value for at least 2 of traps analyzed, which must be at least 50% greater than the highest blank level observed. Levels have been corrected for blanks.

TABLE 13
NON-SILOXANE VAPOR PHASE COMPOUNDS PRESENT IN MOTOR EXHAUSTS AT CONCENTRATIONS GREATER THAN 10 $\mu g/m^3$ in ASCF CHAMBER

Component Concentration, $\mu g/m^3$	Composition[a]	Maximum
Benzene	D,H	17.6
Methylcrotonate	H	15.3
Toluene	H	10.5
Cyanobenzene	H	18.0
C_3-cyclopentane	H	16.1
tri methyl-cyclobutanone	Q	23.5

[a] Composition only listed if present at $>10\mu g/m^3$ in that particular exhaust atmosphere.

from this that the levels of trace organic vapor phase constituents are probably not of concern from a health risk standpoint under most conceivable use scenarios. Only by repeated firings from an enclosed space could these materials reach toxic levels. And before toxic levels of the organic vapor phase species was reached, CO levels would probably be lethal.

Determination of the higher molecular weight particulate-phase constituents proved difficult for the samples from the initial runs of Composition D (the first propellant studied). Because of filter clogging immediately following the firing of the test motors, the number of particles collected was very small. For example, the largest amount of sample collected on any of the initial runs was 40 mg. This was dispersed over a 4"-diameter Teflon-coated glass fiber filter. Initial GC analysis of the extracts indicated very low levels of hydrocarbons. Next, the extracts were subjected to GC/MS analysis with selected ion monitoring (SIM). SIM has the advantage of identifying species from selected characteristic ions, as opposed to using the entire ionic fragmentation pattern. Due to the small amounts of material collected on the filters, quantities detected in the particulate filter extracts were considerably below our normal detection limits for the target constituents. For that reason, in the preceding studies, the particulate collection system was modified to be a two-stage filter. This approach proved to be much more successful at collecting greater amounts of particles. In Table 14 are listed the polynuclear aromatic hydrocarbons (PAH's) determined in the exhaust particles collected from the firings of Compositions D, H, L, and Q. In addition, a comparison is also made between these levels and those determined for outside air at a military base. A few comments are in order. First, only data for particles collected in the coarse filters are reported. The fine filters collected very few particles (1 - 5 mg), and thus many of the levels determined are at or near the instrumental limits of detection. Nitro-PAHs were determined only for Composition D and H exhausts. The levels

Table 14

Concentrations (μg/g) of Nitro-PAH and PAH in Particulate Matter Collected on Coarse Filters at ASCF: Comparison with Outdoor Air Particulate Collected at U.S. Army installation

Constituent	Propellant Exhaust									Ft. Carson[a] Outside Air Particulates
	Composition D		Composition H			Composition L		Composition Q		
	Run 5	Run 6	Run 1	Run 3	Run 4	Run 1	Run 2	Run 1	Run 2	
2-nitrofluorene	BMDL	BMDL	0.039	0.061	0.032	ND	ND	ND	ND	BMDL
9-nitroanthracene	0.14	BMDL	BMDL	BMDL	BMDL	ND	ND	ND	ND	BMDL
1-nitropyrene	BMDL	BMDL	BMDL	BMDL	BMDL	ND	ND	ND	ND	BMDL
benz(a)anthracene	0.22	0.19	0.19	0.15	0.15	0.22	0.19	1.40	0.81	4.9
chrysene	0.26	0.83	0.55	0.61	0.40	0.05	BMDL	4.70	2.28	11.5
benzo(b+j+k)fluoranthrene	0.47	1.7	1.1	1.4	1.1	0.04	0.13	1.60	0.75	15.7
benzo(e)pyrene	0.26	0.66	0.82	0.92	0.86	1.18	0.44	1.40	0.54	9.4
benzo(a)pyrene	0.39	0.31	0.59	0.52	0.37	0.05	BMDL	1.30	0.41	8.0
3-methylcholanthrene	BMDL	BMDL	BMDL	BMDL	BMDL	BMDL	BMDL	0.54	BMDL	BMDL
dibenz(a,j)anthracene	0.13	1.9	0.51	0.52	0.15	0.24	0.14	2.10	1.06	3.7
indeno[1,2,3-cd]pyrene	0.47	0.83	1.4	0.69	0.69	1.74	0.64	1.70	1.06	17
dibenz(a,h)anthracene	0.13	BMDL	0.23	0.16	0.14	0.13	0.31	5.80	1.63	3.9
benzo(g,h,i)perylene	2.0	BMDL	3.2	3.2	BMDL	5.17	1.39	3.80	1.87	21.8

ND: Not detected BMDL: Below method detection limit

[a] Data from Griest, et al., 1988

determined in these earlier studies were so low that a repeat of the complex analyses did not seem warranted. Despite the very low levels of PAH found in the particulates, the results are fairly consistent from sample to sample. The concentrations of a few selected PAHs in the particles of the Q exhaust were somewhat higher, but not by more than an order of magnitude. The only nitro-PAH which was identified consistently in the exhausts of the motors was 2-nitrofluorene, in the exhaust of Composition H. Its concentration ranged from ca. 30 - 60 ng/g. Most of the other PAHs identified and quantified in the exhausts were present at levels less than 1 $\mu g/g$. The outdoor air particulate sample with which a comparison is made was acquired outside a large motor pool building at Fort Carson, Colorado, in the mid-1980's as background data for another project supported by the USABRDL[23]. A major contributor to the particulates in this sample was expected to be diesel- and gasoline-powered motor vehicle exhaust. The comparison indicates that, with the exception of 2-nitrofluorene, the PAH content of the rocket exhaust particulate is substantially less than (usually by a factor of 10 or so) that of outdoor air particulate matter found in a semi-urban setting at a military base. Also, the BaP content of the exhaust particulates is about half that of cigarette smoke particulate matter[24]. Because of the relatively low concentrations of the PAH in the particle phase, the airborne concentrations of the PAHs are very low. For example, at the maximum particle concentration of [illegible] mg/m^3 in the ASCF chamber (as a surrogate for human exposure conditions), the highest observed airborne benzo(a)pyrene concentrations would be approximately 0.09 $\mu g/m^3$, and that of benzo(g,h,i)perylene would be 0.36 $\mu g/m^3$. At these levels, the airborne PAHs and nitro-PAHs in the rocket exhaust probably do not represent an additional health hazard above that of normal urban air particulates for the troops using such weapon systems.

SUMMARY AND RECOMMENDATIONS - PART 1

The exhaust products from the firing of 2x2 rocket motors in a 20 m^3 test chamber have been characterized. The data indicated that of all of the toxic and/or carcinogenic species present, most were present at very low levels. Of the major toxic constituents, carbon monoxide was the most universally present. Interestingly, the formulation with the greatest fraction of inorganic material (Composition L) yielded the highest concentration of CO in the ASCF chamber per 100 g of propellant. Nitric oxide was present in all of the exhausts, but typically at levels less than 5 ppm in the 20 m^3 chamber. No ammonia or hydrogen cyanide was observed at levels greater than 1 ppm. Levels of HCl were observed in the Composition L exhaust which were very high ($>$100 ppm), and it seems likely that firing of this propellant in an enclosed space would produce very high concentrations of this toxic species. However, no data was obtained as to whether the HCl was present in the particle or the vapor phase.

Particles were present at substantial levels in all of the exhaust atmospheres ($\geq$30 mg/m^3). Particle size distributions indicated that for those particles which could be collected under the sampling conditions employed, virtually all of the material was within an inhalable size range ($<$10 μm mass median diameter). A large fraction of the airborne particles were comprised of metallic species. Copper and lead (especially the latter) were present in the ASCF atmospheres of many of the motor types at levels above those regulated by OSHA.

However, the levels of PAHs and nitro-PAHs in the particulates were very low. Comparison with airborne particulate matter collected at a military installation indicated that the PAH content of the particles was about 1/10 that of outdoor air particles.

Quantitative determination of the organic vapor phase constituents was very difficult due to both the very low levels at which they were present and the presence of large amounts of other species in the background samples. The latter included a large number of cyclosiloxanes, probably from the off-gassing of the chamber walls following cleaning. Only a few exhaust components were found at levels greater than a few ppb. These included benzene, toluene, methylcrotonate, and cyanobenzene. These were typically present at levels less than 10 ppb in the chamber.

From the standpoint of follow-on studies, recommendations depend on the goal of such efforts. If the goal is to refine the comparison between the observed chemistry and the predicted compositions, then the determination of methane (CH_4) and molecular hydrogen (H_2) would be very desirable. Such is a very difficult task, and would likely require a dedicated real time mass spectrometer to make such measurements. However, the determination of such constituents would not significantly further the understanding of potential health risks of the exhaust products, since neither are toxic species.

Since these experimental studies were performed, there have been two developments in the field of analytical chemistry which, if applied to these studies, could significantly improve the quality of the data generated, especially with regard to the determination of volatile organics. First, a number of carbon based adsorbents are now commercially available which have many fewer artifacts than the Tenax used in these studies. Were the sorbent traps used in these studies replaced with the new systems, it is likely that the number of artifacts present in the samples would be significantly reduced, minimizing the complexity of the interpretation of the data. Also, the recent development of direct sampling ion trap mass spectrometry (DSITMS) for the determination of airborne vapor phase constituents is significant. DSITMS could be used to provide determination of a number of volatile species of toxicologic interest in real time, much like an NDIR analyzer provides real time measurement of CO or CO_2. Transportable DSITMS systems are now under development at ORNL for air toxics monitoring at environmental remediation sites, and such technology could be useful for other scenarios.

Finally, the most important recommendation for future work is the determination of the exhaust product composition under actual field conditions, firing full scale motors. There are two important reasons for this. First, the data in this study indicates that changes in the physical properties such as burn time can have a radical effect on exhaust composition. This suggests that it will be difficult to obtain highly realistic data unless true field measurements can be made. Secondly, firing of the test motors in an enclosed chamber causes significant run-to-run background contamination problems. Perhaps the firing of motors in single use, disposable structures, such as large nylon tents, would eliminate much of the contamination problem.

PART 2 - MODELING FOR HEALTH HAZARD PREDICTION

INTRODUCTION

Over the past 30 years, several digital computer programs have been developed at the National Aeronautics and Space Administration's Lewis Research Center to carry out the considerable numerical calculations involved in the determination of the equilibrium composition of complex chemical mixtures at high temperatures[25, 26,27]. Updates to these programs have incorporated improved computational methods and adaptations to improvements in computer speeds and capacities. In accordance with a suggestion from project management, we have used the 1986 version[28] of the program described in Reference 27 to obtain estimates of the composition of the exhaust gases from four different solid propellants. This was referred to as the NASA-Lewis model, version CET-86. The program obtains estimates of the equilibrium composition of a mixture of several components by minimizing either the Gibbs function or the Helmholtz function. If temperature and volume are constant, the Helmholtz function of a system decreases during an irreversible process, becoming a minimum at equilibrium; if temperature and pressure are constant, the same is true of the Gibbs function[28]. All gases are assumed to be ideal, even if small amounts of condensed species are present. Calculations can be done for any one of six combinations of assigned state parameters (e.g., temperature, pressure, density, entropy, and enthalpy); additionally, theoretical rocket performance data can be obtained. The assumptions involved in the calculation of rocket performance parameters are listed in Ref. 3. Briefly, they are: (1) validity of the one-dimensional form of the continuity, energy, and momentum equations; (2) zero velocity (no gas movement) in the combustion chamber; (3) complete combustion (in the sense that all reactants are converted to products); (4) adiabatic combustion; (5) isentropic (adiabatic and reversible) expansion; (6) homogeneous mixing; (7) ideal gas law; and (8) zero temperature and pressure lags between condensed and gaseous species. An extensive discussion of these assumptions and their validity can be found in Reference 30.

The program first determines combustion properties in the rocket motor chamber and then determines exhaust composition and properties at various stations in the nozzle. Since our propellants were fired in motors having a range of exit diameters, we used the feature of the program that allows estimation of exit compositions for a set of several exit to throat area ratios. (In this case, the throat of the motor is considered to be the choke point, or opening of the smallest diameter. The exit is the exit of the motor nozzle. Using these definitions, the ratio of the exit:throat areas, A_e/A_t, must always be larger than 1.0.) In Table 15 are listed the ranges of exit/throat area ratios possible for each motor. In each of the predictions, we used the design pressure as the combustion chamber pressure. The throat pressure is defined to be the pressure at which the flow velocity is equal to the velocity of sound.

The iterative procedures used by the program are discussed in detail in Reference 27. Briefly, combustion temperature and equilibrium compositions are determined for an

TABLE 15

EXIT/THROAT AREA RATIO RANGES
TEST MOTOR CONFIGURATIONS

COMPOSITION	MINIMUM THROAT DIAMETER, INCHES	MAXIMUM THROAT DIAMETER, INCHES	NOMINAL EXIT* DIAMETER, INCHES	MINIMUM A_e/A_t	MAXIMUM A_e/A_t	NOMINAL A_e/A_t
D	0.50	0.707	1.0	1.125	6.25	4
H	0.261	0.261	1.0	8.26	22.94	14.7
L	0.28	0.28	1.0	7.17	19.93	12.76
Q	0.188	0.197	1.125	14.49	44.21	35.06

* These are estimated exit diameters. Actual exit diameters varied between 0.75 and 1.25 inches.

assigned chamber pressure and the reactant enthalpy. From the combustion compositions and temperature, the combustion entropy can be determined. Assuming isentropic expansion, the program then obtains a first estimate for the ratio of chamber pressure to throat pressure; from the throat pressure and the entropy, the actual gas velocity, the speed of sound, and the Mach number can be calculated; if the Mach number is not sufficiently close to unity, the pressure ratio is corrected and a further calculation of Mach number is done. Exit conditions for assigned exit-to-throat area ratios are also obtained from an initial estimate of the ratio of the chamber pressure to the exit pressure, followed by iterative correction. The converged value of pressure ratio for each area ratio is used as the initial estimate for the next area ratio.

We obtained the program, test case input, and output from the NASA Lewis Research Center[28]. We were able to compile the program on our VAX 6000-420 computer and were able to reproduce the test case output with no problems. In our series of calculations the program has performed in a very reliable manner; we have had no difficulties with any of the iterative procedures failing to converge.

RESULTS AND DISCUSSION

In Tables 16 - 19 are listed the predicted mole fractions of various exhaust components over the range of potential ratios of exit areas to throat areas. (The full computer printouts for selected runs for each composition are included in Appendix C.) Note that there have been two independent checks of these computations[31]. First, CET86 computations of mole fractions of Composition H were checked against the "Blake" code and found to be in excellent agreement. (See discussion regarding Table 23, below). Secondly, the calculations were verified by running MUCET, a modified version of CET86 prepared by Eli Freedman & Associates for use with microcomputers. Results were identical to those reported here.

The model has a cut-off feature. Essentially, it can predict the levels of over 100 compounds, but will only report out those mole fractions which are larger than a user-specified value. For this work, a mole fraction of 5×10^{-7} was employed. The rationale for using this value was as follows. If it is assumed that there are about 2 moles of exhaust products in the ASCF chamber following a firing, a mole fraction of 5×10^{-7} would be equivalent to 1×10^{-6} moles of the particular product in the chamber. This assumption was in fact supported by the chemical characterization data (see above). For a compound with a nominal molecular weight of 100 g/mole, this translates to a concentration of 5 μg/m^3, or 1.5 ppbv, in the 20 m^3 ASCF chamber. Few airborne compounds are considered to be a significant health risk at such low concentrations. In addition, unless a very large sample is acquired, it is usually difficult to confidently quantify such species at these low levels.

Using this criterion, with the exception of the metals in the exhaust products, the only compounds which were predicted to be present in the exhaust were carbon monoxide, carbon dioxide, hydrogen, water vapor, ammonia, and methane. In none of the cases did the model predict significant quantities of nitric oxide, despite the fact that NO was observed at levels near to or greater than 1 ppm on each burn.

Table 16

Predicted Mole Fractions as a Function of Exit/Throat Area Ratios

Composition D

Chamber pressure = 2500 psia

A_e/A_t	1.1300	1.8600	2.2500	3.1300	5.1700	6.2500
Exit T, °K	2256.4	1894.1	1788.5	1626.8	1419.6	1355.0
			Mole fractions			
CO	.37059	.35871	.35390	.34478	.32876	.32241
CO_2	.14561	.15759	.16241	.17154	.18756	.19391
H_2	.11245	.12448	.12931	.13844	.15445	.16080
H_2O	.23930	.22754	.22273	.21362	.19760	.19126
Cu(Total)	2.3949×10^{-3}	2.4058×10^{-3}	2.4062×10^{-3}	2.4063×10^{-3}	2.4063×10^{-3}	2.4062×10^{-3}
Pb(Total)	2.2823×10^{-3}	2.3222×10^{-3}	2.3276×10^{-3}	2.3325×10^{-3}	2.3352×10^{-3}	2.3363×10^{-3}
NH_3	1.1109×10^{-5}	8.7647×10^{-6}	8.4223×10^{-6}	8.2080×10^{-6}	8.6068×10^{-6}	8.8299×10^{-6}
CO/CO_2	2.545	2.276	2.179	2.010	1.753	1.663
NH_3/CO_2	7.629×10^{-5}	5.562×10^{-5}	5.562×10^{-5}	4.785×10^{-5}	4.589×10^{-5}	4.554×10^{-5}
			Chamber pressure = 3000 psia			
A_e/A_t	1.1300	1.8600	2.2500	3.1300	5.1700	6.2500
Exit T, °K	2256.8	1893.7	1788.1	1626.4	1420.8	1355.7
			Mole fractions			
CO	.37061	.35869	.35388	.34475	.32888	.32248
CO_2	14560	.15761	.16243	.17156	.18744	.19384
H_2	.11245	.12450	.12933	.13846	.15433	.16073
H_2O	.23933	.22752	.22271	.21359	.19772	.19133
Cu(Total)	2.3968×10^{-3}	2.4059×10^{-3}	2.4062×10^{-3}	2.4634×10^{-3}	2.4062×10^{-3}	2.4063×10^{-3}
Pb(Total)	2.2819×10^{-3}	2.3219×10^{-3}	2.3274×10^{-3}	2.3322×10^{-3}	2.3355×10^{-3}	2.3365×10^{-3}
NH_3	1.3315×10^{-5}	1.0519×10^{-5}	1.0110×10^{-5}	9.8554×10^{-6}	1.0279×10^{-5}	1.0565×10^{-5}
CO/CO_2	2.545	2.276	2.179	2.010	1.755	1.664
NH_3/CO_2	9.145×10^{-5}	6.674×10^{-5}	6.224×10^{-5}	5.745×10^{-5}	5.464×10^{-5}	5.450×10^{-5}

A_e/A_t: Ratio of the exit area to throat area

Table 17
Predicted Mole Fractions as a Function of Exit/Throat Area Ratios

Composition H

Chamber pressure = 5000 psia

A_e/A_t	8.3000	10.000	15.000	23.000
Exit T, °K	1575.0	1507.1	1372.2	1251.4
Mole fractions				
CO	.25795	.25360	.24311	.23079
CO_2	.25776	.26229	.27332	.28608
H_2	8.5609×10^{-2}	9.0087×10^{-2}	.10095	.11357
H_2O	.24704	.24278	.23242	.22018
HCl	4.5892×10^{-4}	3.4824×10^{-4}	1.8022×10^{-4}	8.1443×10^{-5}
KCl	1.3356×10^{-2}	1.2799×10^{-2}	1.0928×10^{-2}	7.7913×10^{-3}
KCl(l)[a]	0.0000 0	0.0000 0	0.0000 0	1.5516×10^{-3}
NH_3	2.5247×10^{-6}	2.5729×10^{-6}	2.7684×10^{-6}	3.0523×10^{-6}
CO/CO_2	1.0007	.9669	.8895	.8067
HCl/CO_2	1.7804×10^{-3}	1.3277×10^{-3}	6.5937×10^{-4}	2.8469×10^{-4}
NH_3/CO_2	9.7947×10^{-6}	9.8094×10^{-6}	1.0129×10^{-5}	1.0669×10^{-5}

A_e/A_t: Ratio of the exit area to throat area
[a]: Liquid

Table 18
Predicted Mole Fractions as a Function of Exit/Throat Area Ratios

Composition L

Chamber pressure = 2500 psia

A_e/A_t	7.2000	10.000	15.000	20.000
Exit T, °K	1281.3	1175.4	1059.3	986.5
Mole fractions				
CO	.14681	.13536	.11945	.10732
CO_2	.11988	.13129	.14697	.15895
HCl	.20072	.20084	.20139	.20167
H_2O	.25903	.24758	.23169	.21983
Al_2O_3	4.5708×10^{-3}	4.5704×10^{-3}	4.5672×10^{-3}	4.5669×10^{-3}
$BaCl_2$(Total)	4.6571×10^{-4}	4.6849×10^{-4}	4.6850×10^{-4}	4.6849×10^{-4}
Cr_2O_3(s)	8.1900×10^{-4}	8.1892×10^{-4}	8.1835×10^{-4}	8.1831×10^{-4}
Cu(s)	0.0000 0	1.3842×10^{-4}	8.3239×10^{-4}	1.1224×10^{-3}
NH_3	9.6149×10^{-6}	1.0736×10^{-5}	1.2947×10^{-5}	1.5182×10^{-5}
CO/CO_2	1.225	1.031	0.813	0.675
HCl/CO_2	1.674	1.530	1.370	1.269
NH_3/CO_2	8.020×10^{-5}	8.177×10^{-5}	8.809×10^{-5}	9.551×10^{-5}

A_e/A_t: Ratio of the exit area to throat area
*: Solid

Table 19
Predicted Mole Fractions as a Function of Exit/Throat Area Ratios

COMPOSITION Q

CHAMBER PRESSURE = 1480 psia

Ae/At	32.600	35.100	35.800
Exit T, °K	918.9	904.4	900.7
Mole Fractions			
CO	2.1030×10^{-1}	2.0683×10^{-1}	2.0590×10^{-1}
CO_2	1.8391×10^{-1}	1.8732×10^{-1}	1.8823×10^{-1}
H_2O	1.0248×10^{-1}	9.9504×10^{-2}	9.8735×10^{-2}
NH_3	1.5108×10^{-5}	1.5668×10^{-5}	1.5810×10^{-5}
ZrO_2 (Total)	2.3203×10^{-3}	2.3216×10^{-3}	2.3220×10^{-3}
Pb	1.0228×10^{-3}	1.0234×10^{-3}	1.0236×10^{-3}
CH_4	7.2073×10^{-4}	1.0005×10^{-3}	1.0889×10^{-3}
Bi	1.0055×10^{-5}	1.3159×10^{-5}	1.3826×10^{-5}
CO/CO_2	1.143	1.102	1.094
NH_3/CO_2	8.215×10^{-5}	8.364×10^{-5}	8.399×20^{-5}

A_e/A_t: Ratio of the exit area to throat area

For many of the input parameters, the model was not particularly sensitive to substantial changes. For example, for Composition H, a nearly 3-fold change in the exit/throat area ratios decreased the predicted mole fraction of CO by less than 12%. The ratio of major components was not significantly altered. For Composition D, a 5-fold change in the A_e/A_t reduced the CO/CO_2 ratio by 35%. The ratios of minor to major components were typically affected to a greater degree. In many cases, mistakes made in the original entry of data into the model were difficult to identify, since the mistaken or modified entry resulted in such a small change in the data output. For example, considerable effort was place into obtaining or calculating the best heats of formation for compounds present in the formulations. However, an exact value may not be particularly critical to the modeling projections. For example, in Table 20 are compared the mole fractions predicted by the model for a ±5% change in the heat of formation of ammonium perchlorate, which comprises nearly 75% of the starting formulation. The results of the manipulation show only minor changes in the predicted mole fractions. For example, the predicted mole fraction of HCl changed only in the fourth decimal place.

From the standpoint of predicting the composition of the exhaust products in the chamber, the model was not particularly effective. As stated previously, in no case did the model predict NO to be present at levels above 10 ppb, even though NO levels were experimentally observed near 1 ppm. In Table 21 are compared the ranges of observed and predicted ratios of carbon monoxide to carbon dioxide in the ASCF chamber. For Composition H, the predicted values were very close to those observed. For Composition L, the model was accurate to within a factor of 2 - 3. For the other two formulations tested, there was substantial disparity between observed and predicted values. In both of these cases, the model predicted a much higher fraction of CO to be present than that which was observed. If the model had been used to make a health risk projection, the risk from CO exposure would have been considerably overestimated.

The comparison of observed and predicted absolute concentration levels in the ASCF chamber is a much more complex task. Briefly, the moles of the elements present in the formulation were computed. Since we did not determine water vapor or hydrogen gas in the chemical characterization studies, it was assumed that all of the H present in the formulation was converted to water vapor. (From a functional standpoint of predicting the concentrations of other species, it makes no difference if the H present existed as water vapor or H_2 gas.) Next, the total number of moles measured in the chamber was calculated, assuming 100% efficiency of conversion of H to water in the chamber. Finally, the mole fractions of the various species were multiplied by the total number of moles present, and divided by the chamber volume, in order to estimate chamber concentrations of the target species. The results of these calculations are summarized in Table 22. In general, the model was very good at predicting the concentrations of metallic species. In the case of zirconium oxide for Composition Q, and copper for Composition D, there was substantial over-estimation of the concentrations. This may be due to settling of particulates containing

TABLE 20
Effect of ± 5% Shift in Heat of Formation of Ammonium Perchlorate
Composition L

Predicted Mole Fractions

H_f = -74109. cal/mole				
A_e/A_t	7.2	10.0	15.0	20.0
Predicted Temperature, °K	1248.8	1146.3	1033.7	963.8
CO	.14393	.13194	.11561	.10325
CO_2	.12259	.13431	.15041	.16255
CO/CO_2	1.17	.98	.77	.64
H_2O	.25526	.24320	.22699	.21523
H_2	.19284	.20402	.21948	.23066
HCl	.19924	.19992	.20044	.20076
N_2	7.833×10^{-2}	7.826×10^{-2}	7.822×10^{-2}	7.823×10^{-2}
Cu(s)	1.583×10^{-3}	2.442×10^{-3}	3.070×10^{-3}	3.331×10^{-3}
NH_3	1.143×10^{-5}	1.284×10^{-5}	1.566×10^{-5}	1.836×10^{-5}
H_f = -67051. cal/mole				
A_e/A_t	7.2	10.0	15.0	20.0
Predicted Temperature, °K	1300.9	1194.0	1075.7	1001.2
CO	.14912	.13778	.12215	.11017
CO_2	.11748	.12854	.14394	.15578
CO/CO_2	1.27	1.07	.85	.71
H_2O	.26048	.24902	.23337	.22157
H_2	.18794	.19841	.21330	.22469
HCl	.19898	.19975	.20032	.20059
N_2	7.836×10^{-2}	7.827×10^{-2}	7.821×10^{-2}	7.820×10^{-2}
Cu(s)	1.257×10^{-3}	2.240×10^{-3}	2.958×10^{-3}	3.260×10^{-3}
NH_3	8.885×10^{-6}	9.774×10^{-6}	1.169×10^{-5}	1.367×10^{-5}

A_e/A_t: Ratio of the exit area to throat area

these species before they could be collected. For Compositions D and Q, the model substantially over-predicts CO and underestimates the amount of CO_2 produced. In the cases of the formulations which were expected to produce measurable amounts of HCl, the model predicted more HCl than was measured in both cases: It could be that in this case, the acquisition of the sample could be suspect. First, some of the HCl or potassium chloride could have been adsorbed on particulate matter which settled very rapidly in the chamber. In this case, the material would not reach the input to the continuous HCl analyzer. In addition, some of the HCl may have been lost in the short lengths of Teflon tubing leading from the chamber atmosphere to the analyzer.

TABLE 21

COMPARISON OF OBSERVED AND PREDICTED CARBON MONOXIDE: CARBON DIOXIDE RATIOS

	Observed		Predicted	
Propellant Composition	Minimum	Maximum	Minimum	Maximum
D	0.0924	0.2265	1.663	2.545
H	1.028	1.160	0.8067	1.0007
L	1.817	2.473	0.675	1.225
Q	0.0622	0.0779	1.094	1.143

In terms of the trace organic vapor and particle phase constituents, the model correctly predicts that the concentrations of these species will be low. In fact, the observed levels of such species as benzene and benzo(a)pyrene were much less than 100 ppbv, or 1 $\mu g/m^3$, respectively. However, the number of toxic species which the model considers is limited, and it is certainly conceivable that a compound not considered by the model could be present at sufficiently high levels to warrant some health risk consideration.

LIMITATIONS AND MODIFICATIONS

In addition to not considering all of the toxic species likely to be produced by the ignition of a predominantly organic matrix, the model does have several limitations. First, it is an equilibrium based system, and does not take into account those synthesis pathways which may be governed predominantly by kinetic processes. Secondly, it assumes ideal gas behavior on the part of all of the gases produced. This assumption is not likely to be accurate over the entire range of conditions existing inside the rocket motor. However, from a practical standpoint, this may not be a severe limitation. For example, the magnitude of non-ideal gas effects depends primarily on the density and the temperature in the system. For the system in question, the largest densities occur in the chamber. Interestingly, the most dense gas (H), has a density of only 0.037 g/mL, which is not sufficiently large to induce substantial deviations from the ideal gas law. To illustrate this point, Freedman[31] has used the "Blake" code to compute chamber concentrations (at 340.23 atmospheres pressure and a temperature of 3167° K) assuming both ideal and real gas equations of state. This was performed for Composition H, whose exhaust products were capable of reaching some of the higher temperatures in the study. The results are listed in Table 23. It is clear that the differences between the real and the ideal gaseous equations of state are very small. And although there are differences between the NASA-Lewis results and those from the "Blake" code, the differences are negligible from a practical standpoint and are due to differences in the thermodynamic data bases themselves.

Finally, and probably most importantly, the model assumes that all of the chemical processes are frozen at the point at which the exhaust gases exit the motor. There is a considerable body of evidence to suggest that this is not the case. For example, the model predicts that no significant production of NO will occur for any of the formulations tested. However, NO was in fact observed. We believe that its presence is due to the effect of the heated exhaust gases on the ambient air in the chamber. That is, the heat from the motor firing causes the formation of nitrogen monoxide. The production of NO is probably proportional to the duration of the flame contact with the air. For example, during run No. 5 for Composition D, the shock wave from the firing of the motor caused some damage to the chamber. A different nozzle was installed on the test motor used for burn #6. This lengthened the burn time, and reduced the pressure of the burn. Such resulted in some substantial differences between burns #5 and #6 for the Composition D motors. The change in the NO concentration is considerable. Probably, the increase in time that the flame is in contact with the air causes much more NO to be produced. Note also the change in the CO concentration from Run No. 5 to Run No. 6.

Following consultations with Dr. Eli Freedman, we decided to test the hypothesis that including a step in the computer calculations which would determine the influence of mixing the predicted exhaust gases with ambient air would lead to a more accurate prediction of the observed gas concentrations in the chamber. The model was revised to mix the exhaust gases with the ambient air at fixed ratios and at varying pressures and temperatures. As an example, the exit composition from propellant D (a formula which had initially yielded a relatively inaccurate prediction of the observed CO/CO_2 ratio) was selected as a "fuel" which could be mixed with air. Initial exit pressure and temperature were set at 39.5 atmospheres and 1837 °K, respectively. The "fuel" was mixed with ambient air in the ratios given in Table 24 to yield equilibrium compositions at two arbitrarily selected lower pressures. As indicated in Table 24, there was a substantial decrease in the CO/CO_2 ratio. The resulting ratio is much closer to that which was observed experimentally than the ratio predicted by the unmodified model, suggesting that there is considerable mixture with ambient air and conversion of carbon monoxide to carbon dioxide between the vicinity of the motor exit and the analysis train. That the model does not consider the influence of mixing with ambient

TABLE 22

COMPARISON OF OBSERVED AND PREDICTED* CONCENTRATIONS
OF EXHAUST CONSTITUENTS IN ASCF CHAMBER

CONSTITUENT	COMPOSITION D		COMPOSITION H		COMPOSITION L		COMPOSITION Q	
	Observed[a]	Predicted	Observed[b]	Predicted	Observed[c]	Predicted	Observed[d]	Predicted
Carbon Monoxide, ppm	282	943	296	240	154	171	84	542
Carbon Dioxide, ppm	1245	538	270	248	344	188	1324	491
NO, ppm	2.2	0[e]	3.7	0[e]	0.75	0[e]	1	0[e]
KCl/HCl, ppm	BMDL	0[e]	<1	14	114	270	BMDL	0[e]
Cu, mg/m^3	4.0	17	BMDL	0[e]	4.5	3.6	0.02	0[e]
Al_2O_3, mg/m^3	BMDL	0[e]	BMDL	0[e]	6.8	6.1	BMDL	0[e]
Pb, mg/m^3	37	55	BMDL	0[e]	16	21.9	BMDL	0[e]
ZrO, mg/m^3	BMDL	0[e]	BMDL	0[e]	<0.1	29.5	BMDL	0[e]

[a] Run #5
[b] Average of Runs 1,3, & 4
[c] Average of Runs 1 - 4
[d] Gaseous components means of Runs 1, 2, 3; Particle component means of Runs 1 & 3
[*] Predicted using assumption that all H in formulation of H_2O during burn. See Text.
[e] Predicted mole fraction of component less than 0.5×10^{-8} cut off.
BMDL: Below Method Detection Limit

TABLE 23

Effect of Choice of Gaseous Equation of State on Computed Mole Fractions for Composition H*

	BLAKE		NASA-Lewis
NAME	IDEAL	REAL	IDEAL
CO	0.2928486	0.2932262	0.29422
H_2O	0.2679565	0.2685877	0.27100
CO_2	0.2183805	0.2180917	0.21722
N_2	0.1346118	0.1346414	0.13459
H_2	4.927155×10^{-2}	4.886758×10^{-2}	4.8588×10^{-2}
HCl	8.636553×10^{-3}	8.599959×10^{-3}	
KOH	7.785912×10^{-3}	7.757804×10^{-3}	
KCl	7.232547×10^{-3}	7.278343×10^{-3}	
NO	1.281355×10^{-3}	1.270143×10^{-3}	
O_2	5.792795×10^{-4}	5.639095×10^{-4}	
NH_3	8.57131×10^{-6}	8.776596×10^{-6}	
CH_2O	2.823712×10^{-6}	2.871074×10^{-6}	
HCN	2.529327×10^{-6}	2.631338×10^{-6}	
Cl_2	2.863636×10^{-7}	2.811794×10^{-7}	
$COCl_2$	2.512875×10^{-10}	2.628192×10^{-10}	
K	1.164592×10^{-3}	1.15023×10^{-3}	8.4006×10^{-4}
COCl	1.79761×10^{-6}	1.84523×10^{-6}	
OH	6.396093×10^{-3}	6.222507×10^{-3}	
KO	5.224935×10^{-5}	5.182151×10^{-5}	
H	3.155921×10^{-3}	3.057469×10^{-3}	
O	2.448266×10^{-4}	2.370879×10^{-4}	
N	1.259862×10^{-6}	1.24317×10^{-6}	
CHO	2.055275×10^{-5}	2.080149×10^{-5}	
Cl	3.638269×10^{-4}	3.574871×10^{-4}	

* From Reference No. 30

air on the products of propellant firing has been observed by other investigators[32]. Snelson, et al. reported that double base propellants fired in Argon atmospheres produced mole fractions of CO which were much closer to those predicted by thermodynamic modeling than when the same propellants were fired in ambient air.

Table 24

Influence of Exhaust Gas Mixing with Air
on Carbon Monoxide/Carbon Dioxide Ratios

Composition D

	Fuel/Air = 5*		
Pressure, atm	39.5	5.0	1.0
Temperature, °K	1837	1300	1000
CO/CO_2	1.44	1.08	0.74
	Fuel/Air = 3*		
Pressure, atm	39.5	5.0	1.0
Temperature, °K	1837	1300	1000
CO/CO_2	1.16	0.88	0.61
	Fuel/Air = 1*		
Pressure, atm	39.5	5.0	1.0
Temperature, °K	1837	1300	1000
CO/CO_2	0.31	0.25	0.17

* Considers exhaust gases from motor nozzle as "fuel."

RECOMMENDATIONS FOR FURTHER WORK

It would be interesting to compare these results with other computer models. Software is available with similar, but not identical methods of computation and data fitting[33].

It may be possible to extend the NASA Lewis model to account for nonideal gas equations of state for some of the major components, without involving major modifications to the program. However, any revision is not to be undertaken lightly; the program is some 5000 lines of Fortran and represents a very large investment of time and effort. The development of a new model would require a similar investment.

A thorough review of the thermal and transport property data base may seem to be desirable, in order to incorporate any new information available since the 1986 revision, and to have some additional assurance that the data have been entered correctly. However, there have only been 8 changes to the data base, and none have practical significance for this study[31]. And since transport properties are not a significant factor in this work, any changes should not have an effect on the conclusions.

It would be useful to model the chemical kinetics of these processes, using the software described in Reference 34. It should be noted, however, that a considerable amount of effort would be required to elucidate the reactions occurring in these events and to make estimates of the necessary rate constants. The Arrhenius constants and the activation energies for the hundreds of conversions processes are not available. In contrast, modeling the flow processes may be useful, since it could lead to a better understanding of the amount of air entrained with the exhaust during combustion.

It might be useful to do some experimental firings of the motors into inert atmospheres, such as argon, in order to test the air mixing hypothesis. However, such in and of itself would not aid in the refinement of the model.

Finally, alternatives to the "air entrainment" explanation as the source of disagreement between experiment and computation should be explored. For example, calculations described in this report were carried out for two possible cases: either the chemical reactions in the expanding flow from the combustion chamber maintain complete equilibrium from throat to the nozzle exit, or else the flow is completely frozen once it leaves the nozzle throat. But the intermediate case is also possible. That is, the flow may freeze somewhere between the throat and the exit. This could provide a possible explanation for the discrepancy between experiment and computation without requiring the assumption of entrained air. To implement such an approach, an adiabatic expansion calculation should be run. Initial estimates provided to the authors of this report suggest that this approach is feasible[31]. However, to take full advantage of such an approach, careful experimental determination of hydrogen and methane would have to be performed. Because of the complexities of such real time analyses, these measurements could not be performed.

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Appendix A

Selected Rocket Propellant Formulations

Table A-1

COMPOSITION "D" FORMULATION

Abbreviation	Constituent	Formula	Wt %	ΔH_f^* (kcal/mole)
NC	Nitro Cellulose (12.6% N)	$C_6H_{7.55}O_{9.9}N_{2.45}$	49.0 ± 1.5	169.17
NG	Nitroglycerine	$C_3H_5N_3O_9$	40.6	-88.60
DNPA	Di-n-propyl adipate	$C_{12}H_{12}O_4$	3.0	
NDPA	2-Nitrodiphenyl amine	$C_{12}H_{11}N_2O_2$	2.0 ± 0.05	-16.71
	LC-12-6[a]	See note	5.3	
Wax	Candelilla wax	$C_{25}H_{48}O$	0.1	

[a] LC-12-6 is a mixture, consisting of 11.4% Copper, 36% Lead, 40.1% β-resorcylic acid ($C_7H_6O_4$) ($\Delta H_f° = 190$ kcal/mole), and 12.5% 2-hydroxybenzoic acid ($C_7H_6O_3$, $\Delta H_f^* = -141$ kcal/mole)

[*] Heat of formation unavailable

Table A-2

COMPOSITION "H" FORMULATION

Abbreviation	Constituent	Formula	Wt %	$\Delta H_f°$ (kcal/mole)
$KClO_4$	Potassium perchlorate	$KClO_4$	7.8-8.05	-103.43
NC	Nitrocellulose	$C_{12}H_{15}N_5O_{20}$	54.60	169.17
NG	Nitroglycerine	$C_3H_5N_3O_4$	35.50	-88.6
EC	Ethyl Centralite	$C_{17}H_{20}N_2O$	0.9 - 0.8	-25.1
C	Carbon Black	C	1.20	Ref.

The entry "Ref." in the heat of formulation column means that this is a reference element in the NASA-Lewis program.

Table A-3

COMPOSITION "L" FORMULATION

Abbreviation	Constituent	Formula	Wt. %	$\Delta H_f°$ (kcal/mole)
AP	Ammonium Perchlorate	$NH_4 ClO_4$	73.93	-70.58
PVC	Polyvinyl Chloride	$(C_2 H_3 Cl)$	11.67	8.41
DEHA	Di (2-ethyl hexyl) adipate	$C_{22} H_{42} O_4$	11.67	-308.0
CUCR	Copper chromite	$Cu_2 Cr_2 O_4$	0.97	Ref.
A1	Aluminum Powder	Al	0.99	Ref.
C	Carbon Black	C	0.05	Ref.
BACD	Stabilizer (Barium/Cadmium)	Ba-Cd	0.47	Ref.
SDSS	Sodium dioctyl sulfo succinate	$C_{20} H_{37} O_7$ SNa	0.083	*
GMO	Glycerol monooleate	$C_{21} H_{40} O_4$	0.083	*
PTD	Pentaerythrital dioleate	$C_{41} H_{76} O_6$	0.084	*

* Heat of formation unavailable

Table A-4

PROPELLANT "Q" FORMULATION

	Constituent	Formula	Weight %	ΔH°_f (Kcal/mole)
NG	Nitroglycerine	$C_3H_5N_3O_9$	11.36	-88.60
BTTN	Butane triol trinitrate	$C_4H_7N_3O_9$	11.36	-93.07
HMX	Cyclotetramethylene tetranitramine	$C_4H_8N_8O_8$	66.00	17.93
PGA	Polyglycol adipate	$C_{10}H_{16}O_5$	4.63	-262.9
N-100	Tri-functional isocynate	C_2H_3NO	1.68	-23.55
MNA	N-methyl-p-nitroaniline	$C_7H_8N_2O_2$	0.75	*
4-NDPA	4-nitrodiphenylamine	$C_{12}H_{11}N_2O_2$	0.40	15.4
PCP	Polycaprolactone polyol	$C_6H_8O_7$	0.34	-655.1
NC	Nitrocellulose	$C_{12}H_{15}N_5O_{20}$	0.34	169.17
	Lead Citrate	$Pb_3(C_6H_5O_7)_2$*$3H_2O$	1.50	*
ZrC	Zirconium Carbide	ZrC	1.00	-48.5
C	Carbon Black	C	0.40	Ref.
TPB	Triphenyl bismuth	$Bi(C_6H_5)_3$	0.04	*

The entry "Ref." in the heat of formulation column means that this is a reference element in the NASA-Lewis program

* Heats of formation unavailable

Appendix B

Trace Organic Vapor Phase Constituents Observed In Selected Rocket Exhaust Atmospheres

Table B-1

Concentration of Trace Organic Vapor Phase Constituents in ASCF Chamber*

Compositions D and H

	Concentrations, µg/m³									
		Composition H				Composition D				
CONSTITUENTS	Blank 1	No. 1A	No. 2C	No. 2D	Blank 2	No. 1A	No. 2A	No. 2B	No. 3B	Blank 3
Trichlorofluoromethane						17.7	11.2		10.1	
Methylene chloride				8.91	11.9	9.29	6.39		2.11	
Trichloroethane	0.42	0.79		0.93		0.3	0.4			
Benzene	0.82	12.1	16.6	14.4	0.57	3.95	3.79	49.2	15.8	
Trichloroethylene		0.94		3.14						
Methylcrotonate			3.32	31.4	2.09	6.04	4.39	19.7	3.82	0.75
C[1]-benzene		7.16		17	1.57	1.86	2.44	6.66	2.94	1.02
C[3]-cyclopentane				0.85						
Chlorobenzene		2.9								
C[6]-cyclotrisiloxene	3.7	10.6	34.9	58.2	23.9	15.3	14	22.7	6.59	18.4
C[2]-benzene	0.7		3.85		1.27	1.25	0.48			
C[2]-benzene		4.15		7.22			1.6			
Phenylacetylene		1.62	2.13	[illegible]				3.03	1.71	
Styrene		2.9	3.49	[illegible]						

Table B-1 (Page 2)
Compositions D and H

	Concentrations, $\mu g/m^3$									
		Composition H						Composition D		
CONSTITUENTS	Blank 1	No. 1A	No. 2C	No. 2D	Blank 2	No. 1A	No. 2A	No. 2B	No. 3B	Blank 3
C[2]-benzene						0.56	0.76			
Octane		1.28								
Nonene				2.33						
Nonane				1.15						
Terpinene	1.7			4.67	1.19	0.79				
Terpinene				2						
C[2]-benzene								10.6		
C[3]-benzene		1.17		4.24		0.6				
C[3]-benzene		1.36		6.37						
C[1]-sytrene				1.91		0.56				
Heptene							12		4.83	
Cyanobenzene								28	7.91	
Octene			7.11							
C[3]-benzene		1.09		1.66	0.9	0.51	0.56			
Decene		0.91	1.07	2.5		0.56				

Table B-1 (Page 3)
Compositions D and H

	Concentrations, µg/m^3									
		Composition H				Composition D				
CONSTITUENTS	Blank 1	No. 1A	No. 2C	No. 2D	Blank 2	No. 1A	No. 2A	No. 2B	No. 3B	Blank 3
Decane		0.38		1.49			0.48			1.29
Terpinene		1.02	1.84	2.59	1.12	0.98	0.8			
C[8]-cyclotetrasiloxane	6.22	6.03	30.2	20	0.97	4.65	5.19	18.2	6.15	7.48
Teripene		0.87		1.36				4.24		
C[3]-cyclopentane	2.67	6.03	3.26	4.67	25.4	9.75	5.99		0.66	
C[8]-cyclotetrasiloxane			2.31							
C[3]-benzene								1.89	0.88	
C[3]-benzene		0.72								
C[4]-benzene				0.89						
C[3]-cyclopentane				1.87						8.16
Terpinene										8.84
Undecane		1.06	1.6	1.91	0.68	0.6	0.56		0.53	1.56
C[1]-cyclohexanol	2.07	1.28	2.96	4.67	2.39	1.72				1.02
C[4]-benzene		1.47								
C[3]-cyclopentane					1.19			8.32		0.75
C[10]-cyclopentasiloxane		6.41	1.3	25.9	8.21	5.57	5.19	12.1	3.51	12.9

Table B-1 (Page 4)
Compositions D and H

	Concentrations, µg/m³									
		Composition H				Composition D				
CONSTITUENTS	Blank 1	No. 1A	No. 2C	No. 2D	Blank 2	No. 1A	No. 2A	No. 2B	No. 3B	Blank 3
Naphthalene		2.79	4.44	11		1.49	1.2		7.91	8.84
C[10]-cyclopentasiloxane		2.04								
C[3]-cyclopentane			0.77	1.91						
Dodecane		0.26		1.23						
C[3]-cyclopentane	1.7		1.24	2.16	1.87		5.99	29.5		1.22
C[3]-cyclopentane	7.41	4.9	11.2	2.38						52.4
C[12]-cyclohexasiloxan				0.51	38.8		1.92			
Tridecane				1.4				35.6		
C[12]-cyclohexasiloxane	0.89	0.91	16.6	44.1	4.4	1.35			1.71	8.16
Tetradecane	1.26		0.95	1.66		0.38			0.57	0.75
C[5]-benzoquinone	1.41			1.83						1.91
C[9]-aminophenol	2.3		1.36	2.29				1.89		
Penthdecane										0.68
C[12]-cyclohexasiloxane	4.74	0.64	5.92	21.2	1.72		3.2			4.42
Diethylphthalate					4.18					
C[14]-cycloheptasiloxane						4.04			0.29	

Table B-1 (Page 5)
Compositions D and H

	Concentrations, $\mu g/m^3$									
		Composition H				Composition D				
CONSTITUENTS	Blank 1	No. 1A	No. 2C	No. 2D	Blank 2	No. 1A	No. 2A	No. 2B	No. 3B	Blank 3
Hexadecane		1.17		1.1					0.75	
Diethylphthalate										19.1
Diphenylamine								1.89		1.43
Hexadecene	2.74	0.83	3.97			1.07				
Actadecane	8.15		2.84	1.02						
Heptadecane	1.48		1.18	0.64		0.88				0.95
Nonadecane	2		2.37	1.1						2.65

• Missing values denote compound at levels below method detection limits

Table B-2

Concentration of Trace Organic Vapor Phase Constituents in ASCF Chamber*

Composition L

	RETENTION TIME (min)	SYSTEM BLANK ($\mu g/m^3$)	BLANK 1 ($\mu g/m^3$)	SAMPLE 1 ($\mu g/m^3$)	SAMPLE 2 ($\mu g/m^3$)	SAMPLE 3 ($\mu g/m^3$)	BLANK 2 ($\mu g/m^3$)
argon	0.2	2.420	2.330	4.210	13.200	14.390	
carbon dioxide	3.4	0.720	2.730		7.381	13.460	15.180
trichlorotrifluoroethane	10.1		0.270				
octamethyl-cyclotetrasiloxane	21.0	1.490	0.066	8.570		1.540	
mono- or di-subs. benzene	21.8			0.530			
hydroxy-N-phenyl-acetamide or isomers	24.6			1.290			
trimethylsilane compd	24.7	0.580					
octamethyl-cyclotetrasiloxane	25.8		0.106	5.820	0.217	2.050	0.149
hexamethyl-cyclotrisiloxane	27.9			1.370			
octamethyl-cyclotetrasiloxane	28.5			0.312			
decamethyl-cyclopentasiloxane	29.6			1.926		0.569	
dodemethyl-cyclohexasiloxane	33.4			0.496			
hexamethyl-cyclotrisiloxane	34.0	0.930					
hexamethyl-cyclotrisiloxane	42.3	4.680					

* Missing values denote compound at levels below method detection limits

Table B-3
Trace Organic Vapor Phase Constituents in ASCF Chamber

Composition Q

		Concentrations, $\mu g/m^3$							
Constituents	RET TIME, min	SYSTEM BLANK	BLANK-1	TSTAA-1	TSTAA-2	TSTAB-2	TSTAB-4	TSTAA-3	TSTABL-2
argon	0.2	2.420	1.898		0.750	0.071	1.787		2.881
carbon dioxide	3.4	0.720			1.854				
trichlorotrifluoroethane	10.1					0.018		1.217	
octamethyl-cyclotetrasiloxane	21.0	1.490							
hexamethyl-cyclotrisiloxane	21.3				0.081	0.036	1.168		0.207
hexamethyl-cyclotrisiloxane	22.7						0.043		
hexamethyl-cyclotrisiloxane	23.6						0.044		
trimethylsilane compd	24.7	0.580							
octamethyl-cyclotetrasiloxane	25.8		0.024			0.050	0.506		0.403
hydrocarbon	27.3					0.057			0.402
alkylalcohol	27.3			2.175					
hexamethyl-cyclotrisiloxane	27.9						0.080		
decamethyl-cyclopentasiloxane	29.8					0.012	0.074		0.277
naphthalene	31.8						0.072		
trimethyl-cyclobutanone	31.8		0.058	58.625		0.436		20.924	3.504
hexamethyl-cyclotrisiloxane	34.0	0.930							
octamethyl-cyclotetrasiloxane	38.6						0.080	0.423	
phthalate	39.2			18.200			0.064	7.122	
hexamethyl-cyclotrisiloxane	42.3	4.880							
phthalate	43.9				0.081				

Appendix C

Output from Selected Runs of Computer Model
NASA-Lewis CET-86

Table C-1

NASA - Lewis CET - 86

Output

Composition D

Fri Dec 6 18:32:42 EDT 1991

CHN

COMPD.LAS

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REACTANTS
C    6.0000  H   9.9000  N   7.5500  O   2.4500     0.0000   49.000000    -169170.00  S   298.150   F
C    3.0000  H   9.0000  N   5.0000  O   3.0000     0.0000   48.599998     -88600.00  S   298.150   F
C   12.0000  H   4.0000  N  22.0000      0.0000     0.0000    3.000000    -246000.00  S   298.150   F
C   12.0000  H   2.0000  N  11.0000  O   2.0000     0.0000    2.000000     -14710.00  S   298.150   F
C    7.0600  H   4.0000  N   6.0000      0.0000     0.0000    2.400000    -190000.00  S   298.150   F
C    7.0000  H   3.0000  N   6.0000      0.0000     0.0000    0.660000    -141900.00  S   298.150   F
CU   1.0000      0.0000      0.0000      0.0000     0.0000    0.600000          0.00  S   298.150   F
PB   1.0000      0.0000      0.0000      0.0000     0.0000    1.900000          0.00  S   298.150   F

NAMELISTS
$INPT2
KASE     =        402,
T        = 26*0.00000000E+00,
P        =   2500.000     , 25*0.00000000E+00,
PSIA     = T,
NMNG     = F,
NSQM     = F,
V        = 26*0.00000000E+00,
RHO      =   2500.000     , 25*0.00000000E+00,
ERATIO
OF
FPCT
FA
MIX      = 4    1.090005     ,
TP       = F,
HP       = F,
SP       = F,
TV       = F,
UV       = F,
SV       = F,
RKT      = T,
SHOCK    = F,
DETN     = F,
TRACE    = 5.000000000000000000E-07,
SO       = 0.00000000000000000E+00,
SO       = 0.0000000E+00,
IONS     = F,
IDEBUG   =          0,
PHI      = F,
SIUNIT   = F,
INNG     = F,
TRNSPT   = F,
TRPACC   = 0.99990000000000050     ,
DIF      = F,
NODATA   = F,
U        = 1.00000000000000000E+30,
H        = 1.00000000000000000E+30
$END

NO INPT2 VALUE GIVEN FOR OF, EQRAT, FA, OR FPCT

SPECIES BEING CONSIDERED IN THIS SYSTEM
 J 3/78  C                  J12/67  CH                 J12/72  CH2                J 3/61  FORMALDEHYDE       L 4/85  FORMIC ACID
 J 6/69  CH3                L 9/85  HYDROXYMETHYLENE   L 9/85  METHYLOXIDE        L 5/84  CH4                L 9/85  METHANOL
 J 6/69  CN                 J12/70  HCN RAD            J 6/66  CNN RAD            J 9/65  CO                 J 9/65  CO2
 J12/69  C2                 J 3/67  C2H RAD            J 3/61  ACETYLENE          BUR 84  KETENE             BUR 84  C2H3 RAD
 BUR 84  METHYL CYANIDE     BUR 84  CH3CO RAD          BUR 84  CH2CHO RAD         L 4/85  ETHYLENE           BUR 84  ACETALDEHYDE
 L 4/85  ACETIC ACID        L 4/85  (FORMIC ACID)2     P10/83  ETHYL RAD          BUR 84  ETHYL OXIDE RAD    L 5/84  ETHANE
 BUR 84  AZOMETHANE         BUR 84  ETHANOL            BUR 84  DIMETHYL ETHER     J 3/67  CNC RAD            J 3/61  CYANOGEN
 J 9/64  CCO RAD            J12/69  C3                 OO6/61  C3H3 RAD           BUR 84  CYCLOPROPENE       BUR 84  PROPYNE
 BUR 84  ALLENE             BUR 84  C3H5 RAD           BUR 84  CYCLOPROPANE       L 4/85  PROPYLENE          L 9/85  PROPYLENE OXIDE
 L 9/85  I-PROPYL RAD       L 9/85  N-PROPYL RAD       L 4/85  PROPANE            L 1/84  1-PROPANOL         J 6/68  CARBON SUBOXIDE
 J12/69  C4                 BUR 84  BUTADIYNE          BUR 84  BUTAN-1EN-3YN      P10/85  CYCLOBUTADIENE     BUR 84  2-BUTYNE
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 P 4/84  1,3-BUTADIENE        BUR 84  2-BUTENE TRANS     BUR 84  2-BUTENE CIS         BUR 84  ISOBUTENE           BUR 84  1-BUTENE
 L 4/85  (ACETIC ACID)2       L 9/85  S-BUTYL RAD        P10/83  N-BUTYL RAD          L 9/85  T-BUTYL RAD         L 4/85  ISOBUTANE
 L 4/85  N-BUTANE             J 3/61  CARBON SUBNITRID   J12/69  C5                   P10/85  CYCLOPENTADIENE     P12/52  CYCLOPENTANE
 P12/52  1-PENTENE            P10/83  N-PENTYL RAD       L 5/87  T-PENTYL RAD         P10/85  CH3C(CH3)2CH3       P10/85  PENTANE
 P10/85  ISOPENTANE           BUR 84  HEXATRIYNE         L12/84  PHENYL RAD           L12/84  PHENOXY RAD         L12/84  BENZENE
 L12/84  PHENOL               BUR 84  CYCLOHEXENE        P10/83  N-HEXYL RAD          L 3/86  BENZALDEHYDE        P10/84  TOLUENE
 L 4/87  CRESOL               P12/52  1-HEPTENE          P10/83  N-HEPTYL RAD         P 4/81  N-HEPTANE           P12/52  1-OCTENE
 P10/83  N-OCTYL RAD          P 4/85  OCTANE             P 4/85  ISO-OCTANE           P10/83  N-NONYL RAD         BUR 84  NAPTHLENE
 BUR 84  AZULENE              P10/83  N-DECYL RAD        L12/84  O-BIPHENYL RAD       L12/84  BIPHENYL            L 6/88  JET-A(G)
 L 6/87  BIBENZYL             J 6/77  CU                 J12/77  CUO                  J 9/66  CU2                 J 3/77  H
 L12/69  HCN                  J12/70  HCO RAD            J12/70  HNCO                 RUS 78  HNO                 RUS 78  HNO2
 RUS 78  HNO3                 J 9/78  HO2                J 3/77  H2                   J12/65  H2N2                J 3/79  H2O
 L 3/85  H2O2                 J 3/77  N                  J12/78  NCO                  RUS 78  NH                  RUS 78  NH2
 J 6/77  NH3                  RUS 78  NH2OH              RUS 78  NO                   RUS 78  NO2                 J12/64  NO3
 J 3/77  N2                   RUS 78  N2H2               RUS 78  NH2NO2               RUS 78  N2H4                RUS 78  N2O
 RUS 78  N2O3                 RUS 78  N2O4               RUS 78  N2O5                 RUS 78  N3                  RUS 78  N3H
 J 3/77  O                    J 6/77  OH                 J 3/77  O2                   J 6/61  O3                  J 3/62  PB
 J12/71  PBO                  J 9/63  PB2                J 3/78  C(GR)                P10/80  BENZENE(L)          P10/80  TOLUENE(L)
 P10/80  OCTANE(L)            L 6/88  JET-A(L)           J 6/77  CU(S)                J 6/77  CU(L)               BAR 77  CUCO3(S)
 J12/77  CUO(S)                 4/66  CUO2H2(S)          J12/77  CU2O(S)              J12/77  CU2O(L)             L 3/81  H2O(S)
 J 3/79  H2O(L)               J 3/62  PB(S)              J 3/62  PB(L)                J12/71  PBO(RD)             J12/71  PBO(YW)
 J12/71  PBO(L)               J12/71  PBO2(S)            J12/71  PB3O4(S)
 $RKTINP
 EQL     = T,
 FROZ    = T,
 SUBAR   = 13*0.000000000000000E+00,
 SUPAR   =    1.1390000000000000     ,   1.8660000000000000     ,
   2.2500000000000000     ,   3.1380000000000000     ,   5.1780000000000000     ,
   6.2500000000000000     , 7*0.000000000000000E+00,
 PCP     = 22*0.000000000000000E+00,
 TCEST   =    3800.000     ,
 NFZ     =             1
 $END

OF =    0.000000
                                   EFFECTIVE FUEL          EFFECTIVE OXIDANT          MIXTURE
 ENTHALPY                             HPP(2)                   HPP(1)                  HSUB0
 (KG-MOL)(DEG K)/KG               -0.26761290E+03          0.00000000E+00         -0.26761290E+03

KG-FORM.WT./KG                     BOP(I,2)                 BOP(I,1)                 BO(I)
 C                                 0.28227483E-01           0.00000000E+00           0.28227483E-01
 O                                 0.35316637E-01           0.00000000E+00           0.35316637E-01
 H                                 0.27585951E-01           0.00000000E+00           0.27585951E-01
 N                                 0.99408641E-02           0.00000000E+00           0.99408641E-02
 CU                                0.94268964E-04           0.00000000E+00           0.94268964E-04
 PB                                0.91552358E-04           0.00000000E+00           0.91552358E-04

POINT ITN    T         CO             H2O            H2            N2            CU           PB
   1    19 2731.78  -29.493         -35.812       -17.641       -24.954        -9.390       -16.842
   2     5 2463.72  -30.236         -37.864       -17.819       -25.150        -8.128       -16.193
 ADD CU(L)
   2     3 2469.21  -30.231         -37.847       -17.827       -25.165        -8.599       -16.228
 PC/PT= 1.751478    T =  2469.21
   2     2 2469.87  -30.231         -37.848       -17.827       -25.263        -8.599       -16.219
 PC/PT= 1.782840    T =  2469.87

POINT ITN    T         CO             H2O            H2            N2            CU(L)        PB
   3     4 2264.33  -30.968         -38.212       -17.981       -25.345        -8.265       -15.621
   3     4 2256.32  -30.936         -38.262       -17.987       -25.352        -8.251       -15.595
   3     2 2256.31  -30.936         -38.261       -17.987       -25.352        -8.252       -15.595
   4     6 1880.88  -32.584         -41.865       -18.288       -25.717        -7.552       -14.874
   4     5 1894.84  -32.440         -40.947       -18.269       -25.783        -7.578       -14.139
   4     2 1894.08  -32.440         -40.947       -18.269       -25.783        -7.578       -14.139
   5     5 1782.09  -33.017         -41.993       -18.362       -25.825        -7.347       -13.554
   5     4 1788.55  -32.981         -41.936       -18.357       -25.810        -7.359       -13.586
   6     5 1627.60  -33.933         -43.698       -18.581       -26.013        -6.998       -12.584
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    6     3 1626.83  -33.938         -43.787        -18.582        -26.814         -6.996        -12.578
    7     6 1412.44  -35.532         -46.699        -18.728        -26.322         -6.458        -18.842
 ADD PB(L)
    7     3 1413.68  -35.526         -46.684        -18.723        -26.324         -6.461        -18.985
    7     4 1419.58  -35.474         -46.587        -18.715        -26.314         -6.477        -18.995

PRINT ITN    T       CO              CO2            H2             N2             CU(L)          PB
    8     4 1359.67  -36.813         -64.827        -18.795        -26.424         -6.314        -18.862

PRINT ITN    T       CO              CO2            H2O            N2             CU(L)          PB
    8     3 1354.19  -36.865         -64.958        -47.695        -26.434         -6.299        -18.849
 ADD CU(S)
    8     2 1358.80  -36.845         -64.876        -47.643        -26.443         -6.389        -18.858
 REMOVE CU(L)

PRINT ITN    T       CO              CO2            H2O            N2             CU(S)          PB
    8     2 1354.86  -36.861         -64.943        -47.686        -26.436         -6.383        -18.851
    8     3 1355.84  -36.860         -64.939        -47.683        -26.435         -6.383        -18.851
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THEORETICAL ROCKET PERFORMANCE ASSUMING EQUILIBRIUM COMPOSITION DURING EXPANSION

PC = 2500.0 PSIA
CASE NO 487

	CHEMICAL FORMULA				WT FRACTION (SEE NOTE)	ENERGY CAL/MOL	STATE	TEMP DEG K
FUEL	C 6.00000	O 9.90000	H 7.55000	N 2.45000	0.489217	-169170.290	S	298.15
FUEL	C 3.00000	O 9.00000	H 5.00000	N 3.00000	0.405351	-88600.000	S	298.15
FUEL	C 12.00000	O 4.00000	H 22.00000		0.029952	-246000.000	S	298.15
FUEL	C 13.00000	O 1.00000	H 11.00000	N 2.00000	0.019960	-16718.000	S	298.15
FUEL	C 7.00000	O 4.00000	H 6.00000		0.023962	-190000.000	S	298.15
FUEL	C 7.00000	O 3.83600	H 6.00000		0.006389	-141000.000	S	298.15
FUEL	CU 1.00000				0.005990	0.000	S	298.15
FUEL	PB 1.00000				0.018978	0.000	S	298.15

O/F= 0.0000 PERCENT FUEL= 100.0000 EQUIVALENCE RATIO= 1.5433 PHI= 0.0000

	CHAMBER	THROAT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT
PC/P	1.0000	1.7820	2.9558	7.6287	10.333	17.847	35.065	45.555
P, ATM	170.11	95.460	57.553	22.323	16.463	9.9791	4.8514	3.7343
T, DEG K	2731.0	2469.1	2256.4	1894.1	1780.5	1626.0	1419.6	1353.8
RHO, G/CC	1.9346-2	1.2031-2	7.9469-3	3.6746-3	2.8781-3	1.9127-3	1.0658-3	8.6828-4
H, CAL/G	-531.88	-648.72	-741.65	-894.84	-937.58	-1003.93	-1089.09	-1117.26
U, CAL/G	-744.74	-848.86	-917.83	-1041.14	-1076.49	-1130.27	-1199.32	-1222.39
G, CAL/G	-6734.39	-6254.80	-5864.88	-5194.60	-4998.53	-4697.60	-4312.29	-4193.91
S, CAL/(G)(K)	2.2705	2.2705	2.2705	2.2705	2.2705	2.2705	2.2705	2.2705
M, MOL WT	25.493	25.525	25.566	25.585	25.586	25.587	25.592	25.613
(DLV/DLP)T	-1.00076	-1.00182	-1.00075	-1.00010	-1.00085	-1.00002	-1.00217	-1.00137
(DLV/DLT)P	1.0150	1.0294	1.0131	1.0019	1.0009	1.0003	1.0333	1.0219
CP, CAL/(G)(K)	0.4505	0.4521	0.4347	0.4138	0.4111	0.4088	0.4489	0.4375
GAMMA (S)	1.2163	1.2168	1.2277	1.2320	1.2334	1.2347	1.2233	1.2252
SON VEL,M/SEC	1041.0	989.1	947.6	878.8	846.7	887.9	751.1	734.1
MACH NUMBER	0.000	1.000	1.398	1.999	2.176	2.460	2.875	3.015

PERFORMANCE PARAMETERS

AE/AT	1.0000	1.1300	1.8600	2.2500	3.1300	5.2700	6.2500
CSTAR, FT/SEC	4752	4752	4752	4752	4752	4752	4752
CF	0.683	0.915	1.202	1.272	1.372	1.491	1.528
IVAC,LB-SEC/LB	183.7	191.6	213.6	220.1	229.8	242.8	246.8
ISP, LB-SEC/LB	100.9	135.1	171.5	187.9	202.7	220.2	225.7

MOLE FRACTIONS

FORMALDEHYDE	3.8024-6	2.2754-6	1.4699-6	6.7396-7	5.3841-7	3.6196-7	2.1354-7	1.7672-7
FORMIC ACID	5.9494-6	3.2789-6	1.9438-6	7.4984-7	5.5565-7	3.4312-7	1.7469-7	1.3735-7
CH4	7.1355-8	7.8490-8	8.0376-8	1.6185-7	2.2956-7	4.7519-7	1.8569-6	3.1498-6
CO	3.7961-1	3.7529-1	3.7059-1	3.5871-1	3.5398-1	3.4478-1	3.2876-1	3.2241-1
CO2	1.3602-1	1.4075-1	1.4561-1	1.5759-1	1.6241-1	1.7154-1	1.8756-1	1.9391-1
CU	2.3248-3	1.4945-3	6.1020-4	6.7881-5	2.8684-5	5.8681-6	4.8357-7	1.4381-7
CUO	5.816 -6	1.266 -6	1.775 -7	1.808 -9	3.167-10	1.339-11	7.199-14	1.001-14
CU2	3.630 -5	2.141 -5	5.333 -6	1.085 -7	3.166 -8	4.000 -9	8.982-11	1.973-11
H	1.5647-3	7.3076-4	3.3758-4	5.4252-5	2.8597-5	8.4845-6	1.1237-6	5.2840-7
HCN	5.3027-6	3.1758-6	2.0618-6	9.6146-7	7.6286-7	5.2932-7	3.2268-7	2.7087-7
HCO RAD	1.0486-5	3.8734-6	1.5055-6	2.0186-7	9.8682-8	2.8838-8	3.8333-9	1.8278-9
HNCO	1.9396-6	1.0240-6	5.8474-7	2.0366-7	1.4487-7	8.2390-8	3.6548-8	2.7135-8
H2	1.0295-1	1.0757-1	1.1245-1	1.2448-1	1.2931-1	1.3844-1	1.5445-1	1.6080-1
H2O	2.4734-1	2.4375-1	2.3930-1	2.2754-1	2.2273-1	2.1367-1	1.9768-1	1.9126-1
NH2	1.075 -6	3.506 -7	1.213 -7	1.264 -8	5.637 -9	1.366 -9	1.446-10	6.268-11
NH3	1.7570-5	1.3476-5	1.1189-5	8.7647-6	8.4223-6	8.2080-6	8.6068-6	8.8299-6
NO	8.964 -5	2.255 -5	5.633 -6	2.348 -7	7.134 -8	8.322 -9	2.473-10	6.487-11

N2	1.2465-1	1.2679-1	1.2684-1	1.2686-1	1.2687-1	1.2687-1	1.2687-1	1.2687-1
O	9.442 -6	1.424 -6	2.255 -7	2.835 -9	5.437-10	2.736-11	2.015-13	3.182-14
OH	1.0157-3	3.3848-4	1.1133-4	8.3416-6	3.2454-6	5.6352-7	3.1721-8	1.0749-8
O2	9.409 -6	1.399 -6	2.018 -7	2.264 -9	4.149-10	1.919-11	1.721-13	1.825-14
PB	2.1624-3	2.2388-3	2.2825-3	2.3222-3	2.3276-3	2.3325-3	2.1430-3	1.3358-3
PBO	1.6835-4	9.4672-5	5.2128-5	1.3092-5	7.7961-6	3.0464-6	6.1760-7	2.1776-7
PB2	1.3451-6	1.1427-6	9.8653-7	7.7679-7	7.3149-7	6.7905-7	5.4596-7	2.0975-7
CU(S)	0.0000 0	0.0000 0	0.0000 0	0.0000 0	0.0000 0	0.0000 0	0.0000 0	2.4061-3
CU(L)	0.0000 0	8.6644-4	1.7847-3	2.3380-3	2.3735-3	2.4004-3	2.4059-3	0.0000 0
PB(L)	0.0000 0	0.0000 0	0.0000 0	0.0000 0	0.0000 0	0.0000 0	1.9223-4	1.0065-3

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.50000E-06 FOR ALL ASSIGNED CONDITIONS

C	CH	CH2	CH3	HYDROXYMETHYLENE	METHYLOXIDE	METHANOL
CN	HCN RAD	CNN RAD	C2	C2H RAD	ACETYLENE	KETENE
C2H3 RAD	METHYL CYANIDE	CH3CO RAD	CH2CHO RAD	ETHYLENE	ACETALDEHYDE	ACETIC ACID
(FORMIC ACID)2	ETHYL RAD	ETHYL OXIDE RAD	ETHANE	AZOMETHANE	ETHANOL	DIMETHYL ETHER
CNC RAD	CYANOGEN	CCN RAD	C3	C3H3 RAD	CYCLOPROPENE	PROPYNE
ALLENE	C3H5 RAD	CYCLOPROPANE	PROPYLENE	PROPYLENE OXIDE	I-PROPYL RAD	N-PROPYL RAD
PROPANE	1-PROPANOL	CARBON SUBOXIDE	C4	BUTADIYNE	BUTAN-1EN-3YN	CYCLOBUTADIENE
2-BUTYNE	1,3-BUTADIENE	2-BUTENE TRANS	2-BUTENE CIS	ISOBUTENE	1-BUTENE	(ACETIC ACID)2
S-BUTYL RAD	N-BUTYL RAD	T-BUTYL RAD	ISOBUTANE	N-BUTANE	CARBON SUBNITRIL	C5
CYCLOPENTADIENE	CYCLOPENTANE	1-PENTENE	N-PENTYL RAD	T-PENTYL RAD	CH3C(CH3)2CH3	PENTANE
ISOPENTANE	HEXATRIYNE	PHENYL RAD	PHENOXY RAD	BENZENE	PHENOL	CYCLOHEXENE
N-HEXYL RAD	BENZALDEHYDE	TOLUENE	CRESOL	1-HEPTENE	N-HEPTYL RAD	N-HEPTANE
1 OCTENE	N-OCTYL RAD	OCTANE	ISO-OCTANE	N-NONYL RAD	NAPTHLENE	AZULENE
N-DECYL RAD	O-BIPHENYL RAD	BIPHENYL	JET-A(G)	BIBENZYL	HNO	HNO2
HNO3	HO2	H2	H2O2	N	NCO	NH
NH2OH	NO2	NO3	N2H2	NH2NO2	N2H4	N2O
N2O3	N2O4	N2O5	N3	N3H	O3	C(GR)
BENZENE(L)	TOLUENE(L)	OCTANE(L)	JET-A(L)	CUCO3(S)	CUO(S)	CUO2H2(S)
CU2O(S)	CU2O(L)	H2O(S)	H2O(L)	PB(S)	PBO(RD)	PBO(YW)
PBO(L)	PBO2(S)	PB3O4(S)				

NOTE WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

THEORETICAL ROCKET PERFORMANCE ASSUMING FROZEN COMPOSITION DURING EXPANSION

PC = 2500.0 PSIA
CASE NO 402

	CHEMICAL FORMULA				WT FRACTION (SEE NOTE)	ENERGY CAL/MOL	STATE	TEMP DEG K
FUEL	C 6.00000	O 9.90000	H 7.55000	N 2.45000	0.489217	-169170.000	S	298.15
FUEL	C 3.00000	O 9.00000	H 5.00000	N 3.00000	0.405351	-88600.000	S	298.15
FUEL	C 12.00000	O 4.00000	H 22.00000		0.029952	-246000.000	S	298.15
FUEL	C 12.00000	O 2.00000	H 11.00000	N 2.00000	0.019968	-16719.000	S	298.15
FUEL	C 7.00000	O 4.00000	H 6.00000		0.023962	-190000.000	S	298.15
FUEL	C 7.00000	O 3.00000	H 6.00000		0.096589	-141000.000	S	298.15
FUEL	CU 1.00000				0.005990	0.000	S	298.15
FUEL	PB 1.00000				0.018973	0.000	S	298.15

O/F= 0.0000 PERCENT FUEL= 100.0000 EQUIVALENCE RATIO= 1.5413 PHI= 0.0000

	CHAMBER	THROAT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT
PC/P	1.0000	1.7914	2.9815	7.7335	10.513	17.442	36.339	47.638
P, ATM	170.11	94.962	57.058	21.997	16.181	9.7532	4.6814	3.5710
T, DEG K	2731.0	2449.3	2223.9	1849.5	1740.9	1573.3	1353.8	1279.4
RHO, G/CC	1.9346-2	1.2063-2	7.9789-3	3.6949-3	2.8876-3	1.9259-3	1.0745-3	8.6712-4
H, CAL/G	-551.00	-649.42	-742.15	-893.11	-936.07	-1001.42	-1085.03	-1112.81
U, CAL/G	-744.74	-848.35	-915.50	-1037.28	-1071.77	-1124.06	-1190.56	-1212.54
G, CAL/G	-6734.39	-6210.69	-5791.48	-5092.55	-4888.81	-4573.64	-4156.96	-4017.73
S, CAL/(G)(K)	2.2705	2.2705	2.2705	2.2705	2.2705	2.2705	2.2705	2.2705
M, MOL WT	25.493	25.493	25.493	25.493	25.493	25.493	25.493	25.493
CP, CAL/(G)(K)	0.4189	0.4137	0.4086	0.3974	0.3934	0.3863	0.3753	0.3711
GAMMA (S)	1.2286	1.2321	1.2358	1.2440	1.2472	1.2528	1.2621	1.2659
SON VEL,M/SEC	1046.3	992.1	946.7	866.3	841.5	801.8	746.5	726.8
MACH NUMBER	0.000	1.000	1.401	2.007	2.186	2.472	2.882	3.034

PERFORMANCE PARAMETERS

AE/AT	1.0000	1.1300	1.8600	2.2500	3.1300	5.1700	6.2500
CSTAR, FT/SEC	4732	4732	4732	4732	4732	4732	4732
CF	0.688	0.920	1.203	1.275	1.374	1.492	1.529
IVAC,LB-SEC/LB	183.3	191.0	212.7	219.8	228.5	240.3	244.1
ISP, LB-SEC/LB	101.2	135.3	177.3	187.6	202.1	219.4	224.8

MOLE FRACTIONS

FORMALDEHYDE	0.00003	FORMIC ACID	0.00001	CO	0.37961	CO2	0.13662
CU	0.00252	CUO	0.00001	CU2	0.00004	H	0.00156
HCN	0.00001	HCO RAD	0.00001	HNCO	0.00000	H2	0.10295
H2O	0.24734	NH2	0.00000	NH3	0.00002	NO	0.00009
N2	0.12465	O	0.00001	OH	0.00102	O2	0.00001
PB	0.00216	PBO	0.00017	PB2	0.00000		

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.50000E-06 FOR ALL ASSIGNED CONDITIONS

C	CH	CH2	CH3	HYDROXYMETHYLENE	METHYLOXIDE	CH4
METHANOL	CN	NCN RAD	CNN RAD	C2	C2H RAD	ACETYLENE
KETENE	C2H3 RAD	METHYL CYANIDE	CH3CO RAD	CH2CHO RAD	ETHYLENE	ACETALDEHYDE
ACETIC ACID	(FORMIC ACID)2	ETHYL RAD	ETHYL OXIDE RAD	ETHANE	AZOMETHANE	ETHANOL
DIMETHYL ETHER	CNC RAD	CYANOGEN	CCO RAD	C3	C3H3 RAD	CYCLOPROPENE
PROPYNE	ALLENE	C3H5 RAD	CYCLOPROPANE	PROPYLENE	PROPYLENE OXIDE	I-PROPYL RAD
N-PROPYL RAD	PROPANE	1-PROPANOL	CARBON SUBOXIDE	C4	BUTADIYNE	BUTAN-1EN-3YN
CYCLOBUTADIENE	2-BUTYNE	1,3-BUTADIENE	2-BUTENE TRANS	2-BUTENE CIS	ISOBUTENE	1-BUTENE
(ACETIC ACID)2	S-BUTYL RAD	N-BUTYL RAD	T-BUTYL RAD	ISOBUTANE	N-BUTANE	CARBON SUBNITRID
C5	CYCLOPENTADIENE	CYCLOPENTANE	1-PENTENE	N-PENTYL RAD	T-PENTYL RAD	CH3C(CH3)2CH3
PENTANE	ISOPENTANE	HEXATRIYNE	PHENYL RAD	PHENOXY RAD	BENZENE	PHENOL

CYCLOHEXENE	N-HEXYL RAD	BENZALDEHYDE	TOLUENE	CRESOL	1-HEPTENE	N-HEPTYL RAD
N-HEPTANE	1-OCTENE	N-OCTYL RAD	OCTANE	ISO-OCTANE	N-NONYL RAD	NAPTHLENE
AZULENE	N-DECYL RAD	O-BIPHENYL RAD	BIPHENYL	JET-A(G)	BIBENZYL	HNO
HNO2	HNO3	HO2	N2H2	N2O2	N	NCO
NH	NH2OH	NO2	NO3	N2H2	NH2NO2	N2H4
N2O	N2O3	N2O4	N2O5	N3	N3H	O3
C(GR)	BENZENE(L)	TOLUENE(L)	OCTANE(L)	JET-A(L)	CU(S)	CU(L)
CUCO3(S)	CUO(S)	CUO2H2(S)	CU2O(S)	CU2O(L)	H2O(S)	H2O(L)
PB(S)	PB(L)	PBO(RD)	PBO(YW)	PBO(L)	PBO2(S)	PB3O4(S)

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

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REACTANTS
C   6.0000  H   9.7800  N   7.5300  N   2.4500      0.0000  49.889000   -167170.00  S   298.150    F
C   3 0000  H   9 0000  N   5.0000  N   3.0000      0.0000  40.399990    -88600.00  S   298.150    F
C  12.0000  H   4.0000  N  22.0000      0.0000      0.0000   3.000000   -246000.00  S   298.150    F
C  12 0000  H   2 0000  N  11 0000  N   2.0300      0.0000   2.000000    -16710.00  S   298.150    F
C   7.0000  H   4 0000  N   6 0000      0.0000      0.0000   2.400000   -190000.00  S   293.150    F
C   7.0000  H   3.0000  N   6.0000      0.0000      2.0000   0.660300   -141000.00  S   298.150    F
CU  1.0000      0.0000      0.0000      0.0000      0.0000   0.680000         3.00  S   298.150    F
PB  1.0000      0.0000      0.0000      0.0000      0.0000   1.900000         0.00  S   298.150    F

NAMELISTS
$INPT2
KASE     =          433,
T        = 26*0 00000000E+00,
P        =    3000.000     , 25*0.0000000E+00,
PSIA     = T,
NMMG     = F,
NSGM     = F,
V        = 26*0.0000000E+00,
RHO      =    3000.000     , 23*0.0000000E+00,
ERATIO   = F,
OF       = F,
FPCT     = F,
FA       = F,
MIX      = 26*-1.000000     ,
TP       = F,
HP       = F,
SP       = F,
TV       = F,
UV       = F,
SV       = F,
RKT      = T,
SHOCK    = F,
DETN     = F,
TRACE    =  5.0000000000000000E-07,
SG       =  2.0000000000000000E-06,
S0       =  0.0000000E+00,
IONS     = F,
IDEBUG   =            0,
PHI      = F,
SIGNIT   = F,
INMG     = F,
TRNSPT   = F,
TRPACC   =  0.9999000000000000     ,
DIF      = F,
NODATA   = F,
U        =  1 0000000000000000E+30,
W        =  1.0000000000000000E+30
$END

NO INPT2 VALUE GIVEN FOR OF, EQRAT, FA, OR FPCT
 $RKTINP
 EQL      = T,
 FROZ     = T,
 SUBAR    = 13*0 0000000000000000E+00,
 SUPAR    =    1.130000000000000     ,    1 600000000000000     ,
   2 250000000000000     ,   3.130000000000000     ,   5.170000000000000     ,
   6.250000000000000     , 7*0 0000000000000000E+00,
 PCP      = 22*0 0000000000000000E+00,
 TCEST    =    3800 000     ,
 NFZ      =            1
 $END

OF =    0 000000
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                                 EFFECTIVE FUEL        EFFECTIVE OXIDANT          MIXTURE
ENTHALPY                             HPP(2)                 HPP(1)                 HSUB0
(KG-MOL)(DEG K)/KG              -0.26761298E+03         0.00000000E+00        -0.26761298E+03

KG-FORM.WT./KG                      BOP(I,2)               BOP(I,1)                B0(I)
 C                               0.20227483E-01         0.00000000E+00         0.20227483E-01
 O                               0.35316637E-01         0.00000000E+00         0.35316637E-01
 H                               0.27585951E-01         0.00000000E+00         0.27585951E-01
 N                               0.99408661E-02         0.00000000E+00         0.99408661E-02
 CU                              0.94268964E-04         0.00000000E+00         0.94268964E-04
 PB                              0.91552358E-04         0.00000000E+00         0.91552358E-04

POINT ITN    T        CO            H2O          H2           N2           CU           PB
   1   10 2733.10  -29.318        -35.626      -17.460      -24.773       -9.221      -16.665
   2    5 2464.89  -30.854        -36.881      -17.638      -24.976       -7.957      -16.813
 ADD CU(L)
   2    3 2471.86  -30.837        -36.859      -17.647      -24.985       -8.682      -16.847
 PC/PT= 1.781930    T =  2471.86
   2    3 2470.79  -30.840        -36.862      -17.648      -24.986       -8.682      -16.846
 PC/PT= 1.783035    T =  2470.79

POINT ITN    T        CO            H2O          H2           N2           CU(L)        PB
   3    4 2264.82  -30.725        -38.828      -17.889      -25.164       -8.266      -15.442
   3    4 2256.71  -30.754        -38.878      -17.806      -25.171       -8.252      -15.415
   3    2 2256.88  -30.754        -38.878      -17.806      -25.171       -8.252      -15.416
   4    6 1880.55  -32.323        -40.885      -18.097      -25.534       -7.551      -13.889
   4    5 1893.65  -32.259        -40.768      -18.087      -25.520       -7.578      -13.954
   4    2 1893.69  -32.259        -40.768      -18.087      -25.520       -7.578      -13.955
   5    5 1782.29  -32.832        -41.816      -18.180      -25.642       -7.345      -13.368
   5    4 1788.13  -32.808        -41.758      -18.175      -25.636       -7.358      -13.401
   6    5 1627.37  -33.752        -43.518      -18.318      -25.838       -6.998      -12.399
   6    3 1626.43  -33.720        -43.529      -18.319      -25.832       -6.995      -12.393
   7    6 1411.95  -35.353        -46.524      -18.538      -26.140       -6.457      -10.655
 ADD PB(L)
   7    3 1414.43  -35.340        -46.492      -18.544      -26.145       -6.464      -10.987
   7    4 1420.85  -35.285        -46.388      -18.535      -26.133       -6.481      -11.001

POINT ITN    T        CO            CO2          H2           N2           CU(L)        PB(L)
   8    4 1360.71  -35.824        -64.611      -18.614      -26.242       -6.317      -10.864

POINT ITN    T        CO            CO2          H2O          N2           CU(L)        PB(L)
   8    3 1354.84  -35.879        -64.762      -47.504      -26.253       -6.300      -10.851
 ADD CU(S)
   8    2 1358.00  -35.862        -64.693      -47.461      -26.268       -6.309      -10.858
 REMOVE CU(L)

POINT ITN    T        CO            CO2          H2O          N2           CU(S)        PB(L)
   8    2 1355.52  -35.875        -64.747      -47.495      -26.255       -6.304      -10.852
   8    3 1355.70  -35.874        -64.742      -47.491      -26.254       -6.305      -10.853
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THEORETICAL ROCKET PERFORMANCE ASSUMING EQUILIBRIUM COMPOSITION DURING EXPANSION

PC = 3000.0 PSIA
CASE NO 403

	CHEMICAL FORMULA				WT FRACTION (SEE NOTE)	ENERGY CAL/MOL	STATE	TEMP DEG K
FUEL	C 6.00000	O 9.90000	H 7.55000	N 2.45000	0.489217	-169178.000	S	298.15
FUEL	C 3.00000	O 9.00000	H 5.00000	N 3.00000	0.405351	-88600.000	S	298.15
FUEL	C 12.00000	O 4.00000	H 22.00000		0.029932	-246000.000	S	298.15
FUEL	C 12.00000	O 2.00000	H 11.00000	N 2.00000	0.019968	-16710.000	S	298.15
FUEL	C 7.00000	O 4.00000	H 6.00000		0.023962	-190806.000	S	298.15
FUEL	C 7.00000	O 3.00000	H 6.00000		0.006589	-141000.000	S	298.15
FUEL	CU 1.00000				0.005998	0.000	S	298.15
FUEL	PB 1.00000				0.018970	0.000	S	298.15

O/F= 0.0000 PERCENT FUEL= 100.0000 EQUIVALENCE RATIO= 1.5413 PHI= 0.0000

	CHAMBER	THROAT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT
PC/P	1.0000	1.7830	2.9579	7.6264	10.361	17.059	35.056	45.558
P, ATM	204.14	114.49	69.014	26.767	19.701	11.967	5.8231	4.4808
T, DEG K	2733.1	2470.5	2256.9	1893.7	1788.1	1626.4	1428.8	1355.7
RHO, G/CC	2.3207-2	1.4423-2	9.5289-3	4.4072-3	3.4425-3	2.2945-3	1.2786-3	1.0319-3
H, CAL/G	-531.60	-640.87	-741.86	-894.25	-937.77	-1004.18	-1089.14	-1117.36
U, CAL/G	-744.02	-841.10	-917.26	-1041.33	-1076.65	-1130.41	-1199.43	-1222.52
G, CAL/G	-6698.53	-6223.77	-5833.91	-5167.01	-4972.36	-4673.03	-4295.02	-4176.24
S, CAL/(G)(K)	2.2563	2.2563	2.2563	2.2563	2.2563	2.2563	2.2563	2.2563
M, MOL WT	25.496	25.542	25.569	25.585	25.586	25.587	25.601	25.619
(DLV/DLP)T	-1.00072	-1.00157	-1.00064	-1.00009	-1.00005	-1.00002	-1.00104	-1.00116
(DLV/DLT)P	1.0146	1.0253	1.0212	1.0016	1.0009	1.0003	1.0282	1.0105
CP, CAL/(G)(K)	0.4402	0.4528	0.4320	0.4134	0.4109	0.4087	0.4426	0.4331
GAMMA (S)	1.2170	1.2181	1.2245	1.2321	1.2335	1.2347	1.2248	1.2264
SON VEL,M/SEC	1041.5	989.8	947.9	878.8	846.6	807.8	751.8	734.6
MACH NUMBER	0.000	1.000	1.399	2.060	2.177	2.461	2.873	3.013

PERFORMANCE PARAMETERS

AE/AT	1.0000	1.1300	1.8600	2.2500	3.1500	5.1700	6.2500
CSTAR, FT/SEC	4753	4753	4753	4753	4753	4753	4753
CF	0.683	0.915	1.202	1.272	1.372	1.491	1.528
IVAC,LB-SEC/LB	183.8	191.6	213.6	228.1	229.8	242.0	246.0
ISP, LB-SEC/LB	100.9	135.2	177.6	187.9	202.7	220.2	225.7

MOLE FRACTIONS

FORMALDEHYDE	4.5635-6	2.7288-6	1.7627-6	8.8834-7	6.3628-7	4.3419-7	2.5605-7	2.1192-7
FORMIC ACID	7.1682-6	3.9252-6	2.3304-6	8.9820-7	6.6629-7	4.1149-7	2.0960-7	1.6482-7
CH4	1.0228-7	1.0863-7	1.1535-7	2.3234-7	3.3141-7	6.0654-7	2.6258-6	4.4849-6
CO	3.7966-1	3.7534-1	3.7061-1	3.5869-1	3.5308-1	3.4475-1	3.2888-1	3.2248-1
CO2	1.3603-1	1.4072-1	1.4560-1	1.5761-1	1.6243-1	1.7156-1	1.8744-1	1.9384-1
CU	2.3119-3	1.2588-3	5.1025-4	5.6316-5	2.3884-5	4.0598-6	3.4421-7	1.2324-7
CUO	5.013 -6	1.075 -6	1.487 -7	1.497 -9	2.619-10	1.105-11	6.251-14	8.549-15
CU2	4.290 -5	1.810 -5	4.464 -6	1.563 -7	4.280 -8	3.971 -9	7.732-11	1.677-11
H	1.4354-3	6.7233-4	3.0003-4	5.1223-5	2.6025-5	7.6443-6	1.0426-6	4.0691-7
HCN	6.3624-6	3.0083-6	2.4714-6	1.1532-6	9.1504-7	6.3498-7	3.0682-7	3.2478-7
HCO RAD	1.1526-5	4.2647-6	1.6511-6	2.2061-7	1.0772-7	3.0620-8	4.2486-9	2.0146-9
HNCO	2.3289-6	1.2291-6	7.0136-7	2.4417-7	1.7369-7	9.9824-8	4.3981-8	3.2639-8
H2	1.0296-1	1.0756-1	1.1245-1	1.2450-1	1.2933-1	1.3846-1	1.5433-1	1.6073-1
H2O	2.4747-1	2.4383-1	2.3933-1	2.2752-1	2.2271-1	2.1359-1	1.9772-1	1.9133-1
NH2	1.180 -6	3.864 -7	1.330 -7	1.301 -8	6.156 -9	1.491 -9	1.605-10	6.910-11
NH3	2.1066-5	1.6133-5	1.3315-5	1.0519-5	1.0118-5	9.8554-6	1.0279-5	1.0565-5
NO	8.246 -5	2.884 -5	5.160 -6	2.134 -7	6.470 -8	7.350 -9	2.319-10	6.125-11

N2	1.2663-1	1.2679-1	1.2684-1	1.2686-1	1.2687-1	1.2687-1	1.2687-1	1.2687-1
O	8.126 -6	1.267 -6	1.890 -7	2.349 -9	4.097-10	7.260-11	1.744-13	2.715-14
OH	9.3335-4	3.1220-4	1.0194-4	7.7732-6	2.9499-6	5.1101-7	2.9613-8	9.9405-9
O2	7.931 -6	1.107 -6	1.491 -7	1.875 -9	3.432-10	1.505-11	1.059-13	1.556-14
PB	2.1627-3	2.2300-3	2.2019-3	2.3219-3	2.3274-3	2.3322-3	1.0094-3	1.1210-3
PBO	1.6927-4	9.5871-5	5.2104-5	1.3067-5	7.7703-6	2.0605-6	5.2704-7	1.0400-7
PBO2	1.6105-6	1.3666-6	1.1020-6	9.3201-7	8.7732-7	6.1586-7	4.6515-7	1.7706-7
CU(S)	0.0000 0	0.0000 0	0.0000 0	0.0000 0	0.0000 0	0.0000 0	0.0000 0	2.4062-3
CU(L)	0.0000 0	1.1891-3	1.0065-3	2.3496-3	2.3824-3	2.4014-3	2.4059-3	0.0000 0
PB(L)	0.0000 0	0.0000 0	0.0000 0	0.0000 0	0.0000 0	0.0000 0	5.2611-4	1.2147-3

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.50000E-06 FOR ALL ASSIGNED CONDITIONS

C	CH	CH2	CH3	HYDROXYMETHYLENE	METHYLOXIDE	METHANOL
CN	HCO RAD	CNN RAD	C2	C2H RAD	ACETYLENE	KETENE
C2H3 RAD	METHYL CYANIDE	CH3CO RAD	CH2CHO RAD	ETHYLENE	ACETALDEHYDE	ACETIC ACID
(FORMIC ACID)2	ETHYL RAD	ETHYL OXIDE RAD	ETHANE	AZOMETHANE	ETHANOL	DIMETHYL ETHER
CNC RAD	CYANOGEN	CCO RAD	C3	C3H3 RAD	CYCLOPROPENE	PROPYNE
ALLENE	C3H5 RAD	CYCLOPROPANE	PROPYLENE	PROPYLENE OXIDE	I-PROPYL RAD	N-PROPYL RAD
PROPANE	1-PROPANOL	CARBON SUBOXIDE	C4	BUTADIYNE	BUTAN-1EN-3YN	CYCLOBUTADIENE
2-BUTYNE	1,3-BUTADIENE	2-BUTENE TRANS	2-BUTENE CIS	ISOBUTENE	1-BUTENE	(ACETIC ACID)2
S-BUTYL RAD	N-BUTYL RAD	T-BUTYL RAD	ISOBUTANE	N-BUTANE	CARBON SUBNITRID	C5
CYCLOPENTADIENE	CYCLOPENTANE	1-PENTENE	N-PENTYL RAD	T-PENTYL RAD	CH3C(CH3)2CH3	PENTANE
ISOPENTANE	HEXATRIYNE	PHENYL RAD	PHENOXY RAD	BENZENE	PHENOL	CYCLOHEXENE
N-HEXYL RAD	BENZALDEHYDE	TOLUENE	CRESOL	1-HEPTENE	N-HEPTYL RAD	N-HEPTANE
1-OCTENE	N-OCTYL RAD	OCTANE	ISO-OCTANE	N-NONYL RAD	NAPTHLENE	AZULENE
N-DECYL RAD	O-BIPHENYL RAD	BIPHENYL	JET-A(G)	DIBENZYL	HNO	HNO2
HNO3	HO2	H2O2	N2O2	N	NCO	NH
NH2OH	NO2	NO3	N2H2	NH2NO2	N2H4	N2O
N2O3	N2O4	N2O5	N3	N3H	O3	C(GR)
BENZENE(L)	TOLUENE(L)	OCTANE(L)	JET-A(L)	CUCO3(S)	CUO(S)	CUO2H2(S)
CU2O(S)	CU2O(L)	H2O(S)	H2O(L)	PB(S)	PBO(RD)	PBO(YW)
PBO(L)	PBO2(S)	PB3O4(S)				

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

THEORETICAL ROCKET PERFORMANCE ASSUMING FROZEN COMPOSITION DURING EXPANSION

PC = 3000.0 PSIA
CASE NO. 403

	CHEMICAL FORMULA				WT FRACTION (SEE NOTE)	ENERGY CAL/MOL	STATE	TEMP DEG K
FUEL	C 6.00000	O 9.96000	H 7.55000	N 2.45000	0.409217	-169170.000	S	298.15
FUEL	C 3.00000	O 9.00000	H 5.00000	N 3.00000	0.405351	-88600.000	S	298.15
FUEL	C 12.00000	O 4.00000	H 22.00000		0.029952	-246000.000	S	298.15
FUEL	C 12.00000	O 2.00000	H 11.00000	N 2.00000	0.019960	-14710.000	S	298.15
FUEL	C 7.00000	O 4.00000	H 6.00000		0.023962	-190000.000	S	298.15
FUEL	C 7.00000	O 3.00000	H 4.00000		0.006589	-141000.000	S	298.15
FUEL	CU 1.00000				0.005990	0.000	S	298.15
FUEL	PB 1.00000				0.010970	0.000	S	298.15

O/F= 0.0000 PERCENT FUEL= 100.0000 EQUIVALENCE RATIO= 1.5413 PHI= 0.0000

	CHAMBER	THROAT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT
PC/P	1.0000	1.7914	2.9813	7.7330	10.512	17.440	36.334	47.631
P, ATM	204.14	113.96	68.471	26.398	19.419	11.705	5.6184	4.2858
T, DEG K	2733.1	2458.6	2225.0	1850.6	1741.9	1574.3	1354.7	1280.3
RHO, G/CC	2.3287-2	1.4449-2	9.5616-3	4.4322-3	3.4630-3	2.3182-3	1.2086-3	1.0481-3
H, CAL/G	-531.80	-649.46	-742.22	-893.24	-936.22	-1001.59	-1085.24	-1113.04
U, CAL/G	-744.82	-840.46	-915.64	-1737.40	-1071.98	-1124.29	-1178.83	-1212.82
G, CAL/G	-6698.53	-6170.78	-5762.58	-5068.76	-4866.58	-4553.61	-4141.91	-4001.69
S, CAL/(G)(K)	2.2563	2.2563	2.2563	2.2563	2.2563	2.2563	2.2563	2.2563
M, MOL WT	25.496	25.496	25.496	25.496	25.496	25.496	25.496	25.496
CP, CAL/(G)(K)	0.4190	0.4130	0.4086	0.3974	0.3934	0.3863	0.3754	0.3711
GAMMA (S)	1.2286	1.2321	1.2357	1.2448	1.2471	1.2527	1.2621	1.2658
SON VEL,M/SEC	1046.4	992.3	946.9	866.4	841.7	801.9	746.7	727.0
MACH NUMBER	0.000	1.000	1.401	2.087	2.186	2.472	2.882	3.034

PERFORMANCE PARAMETERS

AE/AT	1.0000	1.1300	1.8600	2.2500	3.1300	5.1700	6.2500
CSTAR, FT/SEC	4733	4733	4733	4733	4733	4733	4733
CF	0.688	0.920	1.285	1.275	1.374	1.492	1.529
IVAC,LB-SEC/LB	187.3	191.1	212.7	219.1	228.6	240.4	244.2
ISP, LB-SEC/LB	101.2	135.3	177.3	187.6	202.2	219.4	224.9

MOLE FRACTIONS

FORMALDEHYDE	0.02600	FORMIC ACID	0.00001	CO	0.37966	CO2	0.13603
CU	0.00231	CUO	0.00001	CUZ	0.00004	H	0.00144
HCN	0.00001	HCO RAD	0.00001	HNCO	0.00000	H2	0.10296
H2O	0.24767	NH2	0.00000	NH3	0.00032	NO	0.00008
N2	0.12667	O	0.00001	OH	0.00093	O2	0.00001
PB	0.00216	PBO	0.00017	PB2	0.00000		

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.50000E-06 FOR ALL ASSIGNED CONDITIONS

C	CH	CH2	CH3	HYDROXYMETHYLENE	METHYLOXIDE	CH4
METHANOL	CN	HCN RAD	CNN RAD	C2	C2H RAD	ACETYLENE
KETENE	C2H3 RAD	METHYL CYANIDE	CH3CO RAD	CH2CHO RAD	ETHYLENE	ACETALDEHYDE
ACETIC ACID	(FORMIC ACID)2	ETHYL RAD	ETHYL OXIDE RAD	ETHANE	AZOMETHANE	ETHANOL
DIMETHYL ETHER	CNC RAD	CYANOGEN	CCO RAD	C3	C3H3 RAD	CYCLOPROPENE
PROPYNE	ALLENE	C3H5 RAD	CYCLOPROPANE	PROPYLENE	PROPYLENE OXIDE	I-PROPYL RAD
N-PROPYL RAD	PROPANE	1-PROPANOL	CARBON SUBOXIDE	C4	BUTADIYNE	BUTAN-1EN-3YN
CYCLOBUTADIENE	2-BUTYNE	1,3-BUTADIENE	2-BUTENE TRANS	2-BUTENE CIS	ISOBUTENE	1-BUTENE
(ACETIC ACID)2	S-BUTYL RAD	N-BUTYL RAD	T-BUTYL RAD	ISOBUTANE	N-BUTANE	CARBON SUBNITRID
C5	CYCLOPENTADIENE	CYCLOPENTANE	1-PENTENE	N-PENTYL RAD	T-PENTYL RAD	CH3C(CH3)2CH3
PENTANE	ISOPENTANE	HEXATRIYNE	PHENYL RAD	PHENOXY RAD	BENZENE	PHENOL

CYCLOHEXENE	N-HEXYL RAD	BENZALDEHYDE	TOLUENE	CRESOL	1-HEPTENE	N-HEPTYL RAD
N-HEPTANE	1-OCTENE	N-OCTYL RAD	OCTANE	ISO-OCTANE	N-NONYL RAD	NAPTHALENE
AZULENE	N-DECYL RAD	O-BIPHENYL RAD	BIPHENYL	JET-A(G)	DIBENZYL	HNO
HNO2	HNO3	HO2	NH2	H2O2	N	NCO
NH	NH2OH	NO2	NO3	N2H2	NH2NO2	N2H4
N2O	N2O3	N2O4	N2O5	N3	N3H	O3
C(GR)	BENZENE(L)	TOLUENE(L)	OCTANE(L)	JET-A(L)	CU(S)	CU(L)
CUCO3(S)	CUO(S)	CUO2H2(S)	CU2O(S)	CU2O(L)	H2O(S)	H2O(L)
PB(S)	PB(L)	PBO(RD)	PBO(YW)	PBO(L)	PBO2(S)	PB3O4(S)

NOTE WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

Table C-2

NASA - Lewis CET - 86

Output

Composition H

Tue Dec 3 18:16:37 EDT 1991

CHN

COMPH2.LAS

```
REACTANTS
N   1.0000  O   4.0000  CL  1.0000      0.0000      0.0000    7.000000   -103438.00  S   298.150   F
C   6.0000  O   9.9000  H   7.5500  N   2.4200      0.0000   54.599998   -169178.00  S   298.150   F
C   3.0000  O   9.0000  H   5.0000  N   3.0000      0.0000   35.500000    -88600.50  S   298.150   F
C  17.0000  H  20.0000  O   1.0000  N   2.0000      0.0000    0.900000    -25560.00  S   298.150   F
C   1.0000      0.0000      0.0000      0.0000      0.0000    1.200000         0.00      0.000

NAMELISTS
$INPT2
KASE    =        700,
T       = 26*0.0000000E+00, 
P       =    5000.000     , 25*0.0000000E+00,
PSIA    = T,
NMHG    = F,
NSQM    = F,
V       = 26*0.0000000E+00,
RHO     =    5000.000     , 25*0.0000000E+00,
ERATIO  = F,
OF      = F,
FPCT    = F,
FA      = F,
MIX     = 26*-1.000000    ,
TP      = F,
HP      = F,
SP      = F,
TV      = F,
UV      = F,
SV      = F,
RKT     = T,
SHOCK   = F,
DETN    = F,
TRACE   =  5.0000000000000000E-07,
S0      =  0.0000000000000000E+00,
S0      =  0.0000000E+00,
IONS    = F,
IDEBUG  =           0,
PHI     = F,
SIUNIT  = F,
INHG    = F,
TRNSPT  = F,
TRPACC  =  0.9999000000000000     ,
DIF     = F,
NODATA  = F,
U       =  1.0000000000000000E+30,
H       =  1.0000000000000000E+30
$END

NO INPT2 VALUE GIVEN FOR OF, EQRAT, FA, OR FPCT

SPECIES BEING CONSIDERED IN THIS SYSTEM
 J 3/78  C                   J12/69  CCL                 J12/68  CCL2                J 6/70  CCL3                P12/83  CCL4
 J12/67  CH                  RUS 79  CHCL                P 6/81  CHCL3               J12/72  CH2                 P12/82  CH2CL2
 J 3/61  FORMALDEHYDE        L 4/85  FORMIC ACID         J 6/69  CH3                 P12/81  CH3CL               L 9/85  HYDROXYMETHYLENE
 L 9/85  METHYLOXIDE         L 5/84  CH4                 L 9/85  METHANOL            J 6/69  CN                  J12/70  HCN RAD
 J 6/66  CNN RAD             J 9/65  CO                  J12/65  COCL                J 6/61  COCL2               J 9/65  CO2
 J12/69  C2                  J12/68  C2CL2               L10/87  C2CL4               L10/87  C2CL6               J 3/67  C2H RAD
 RUS 79  C2HCL               J 3/61  ACETYLENE           BUR 84  KETENE              BUR 84  C2H3 RAD            BUR 84  METHYL CYANIDE
 BUR 84  CH3CO RAD           BUR 84  CH2CHO RAD          L 4/85  ETHYLENE            BUR 84  ACETALDEHYDE        L 4/85  ACETIC ACID
 L 4/85  (FORMIC ACID)2      P10/83  ETHYL RAD           BUR 84  ETHYL OXIDE RAD     L 5/84  ETHANE              BUR 84  AZOMETHANE
 BUR 84  DIMETHYL ETHER      BUR 84  ETHANOL             J 3/67  CNC RAD             J 3/61  CYANOGEN            J 9/66  CCO RAD
 J12/69  C3                  D04/61  C3H3 RAD            BUR 84  CYCLOPROPENE        BUR 84  PROPYNE             BUR 84  ALLENE
 BUR 84  C3H5 RAD            BUR 84  CYCLOPROPANE        L 4/85  PROPYLENE           L 9/85  PROPYLENE OXIDE     L 9/85  I-PROPYL RAD
 L 9/85  N-PROPYL RAD        L 4/85  PROPANE             L 1/84  1-PROPANOL          J 6/68  CARBON SUBOXIDE     J12/69  C4
 BUR 84  BUTADIYNE           P10/85  CYCLOBUTADIENE      BUR 84  BUTAN-1EN-3YN       P 4/84  1,3-BUTADIENE       BUR 84  2-BUTYNE
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BUR 84  2-BUTENE TRANS      BUR 84  2-BUTENE CIS        BUR 84  ISOBUTENE           BUR 84  1-BUTENE            L 4/85  (ACETIC ACID)2
L 9/85  T-BUTYL RAD         L 9/85  S-BUTYL RAD         P10/83  N-BUTYL RAD         L 4/85  N-BUTANE            L 4/85  ISOBUTANE
J 3/61  CARBON SUBNITRID    J12/69  C5                  P10/85  CYCLOPENTADIENE     P12/52  CYCLOPENTANE        P12/52  1-PENTENE
L 5/87  T-PENTYL RAD        P10/83  N-PENTYL RAD        P10/85  PENTANE             P10/85  ISOPENTANE          P10/85  CH3C(CH3)2CH3
BUR 84  HEXATRIYNE          L12/84  PHENYL RAD          L12/84  PHENOXY RAD         L12/84  BENZENE             L12/84  PHENOL
BUR 84  CYCLOHEXENE         P10/83  N-HEXYL RAD         P10/84  TOLUENE             L 6/87  CRESOL              P12/52  1-HEPTENE
P10/83  N-HEPTYL RAD        P 4/81  N-HEPTANE           P12/52  1-OCTENE            P10/83  N-OCTYL RAD         P 4/85  OCTANE
P 4/85  ISO-OCTANE          P10/83  N-NONYL RAD         BUR 84  NAPTHLENE           BUR 84  AZULENE             P10/83  N-DECYL RAD
L12/84  O-BIPHENYL RAD      L12/84  BIPHENYL            L 6/88  JET-A(G)            J 6/72  CL                  J 6/66  CLCN
J 6/61  CLO                 J 3/61  CLO2                J 9/65  CL2                 J12/65  CL2O                J 3/77  H
L12/69  HCN                 J12/70  HCO RAD             J 9/64  HCL                 J12/70  HNCO                RUS 78  HNO
RUS 78  HNO2                RUS 78  HNO3                J 3/79  HOCL                J 9/78  HO2                 J 3/77  H2
J12/65  H2N2                J 3/79  H2O                 L 5/85  H2O2                J 6/62  K                   J 3/66  KCN
J 3/66  KCL                 J 3/63  KH                  J12/67  KO                  J12/78  KOH                 J12/61  K2
J 3/66  K2C2N2              J 3/66  K2CL2               J12/78  K2O2H2              J 3/77  N                   J12/70  NCO
RUS 78  NH                  RUS 78  NH2                 J 6/77  NH3                 RUS 78  NH2OH               RUS 78  NO
RUS 78  NOCL                RUS 78  NO2                 RUS 78  NO2CL               J12/64  NO3                 J 3/77  N2
RUS 78  N2H2                RUS 78  NH2NO2              RUS 78  N2H4                RUS 78  N2O                 RUS 78  N2O3
RUS 78  N2O4                RUS 78  N2O5                RUS 78  N3                  RUS 78  N3H                 J 3/77  O
J 6/77  OH                  J 3/77  O2                  J 6/61  O3                  J 3/78  C(GR)               P10/80  BENZENE(L)
P10/85  TOLUENE(L)          P10/80  OCTANE(L)           L 8/86  JET-A(L)            L 3/81  H2O(S)              J 3/79  H2O(L)
J12/61  K(S)                J12/61  K(L)                J 3/66  KCN(S)              J 3/66  KCN(L)              J 3/66  KCL(S)
J 3/66  KCL(L)              J12/78  KOH(A)              J12/78  KOH(B)              J12/78  KOH(L)              J 6/71  KO2(S)
J 3/66  K2CO3(S)            J 3/66  K2CO3(L)            J 6/63  K2O(S)              J 9/63  K2O2(S)             BAR73   NH4CL(A)
BAR73   NH4CL(B)
$PRTINP
EQL     = T,
FROZ    = T,
SUBAR   = 13*0.00000000000000000E+00,
SUPAR   =   0.30000000000000000    ,   10.000000000000000    ,
  15.000000000000000    ,   23.000000000000000    , 9*0.00000000000000000E+00,
PCP     = 22*0.00000000000000000E+00,
TCEST   =    3800.000    ,
NFZ     =            1
$END

OF =    0.000000
                              EFFECTIVE FUEL        EFFECTIVE OXIDANT        MIXTURE
ENTHALPY                          HPP(2)                HPP(1)               HSUB0
(KG-MOL)(DEG K)/KG          -0.27006927E+03        0.00000000E+00      -0.27006927E+03

KG-FORM WT./KG                   BOP(I,2)              BOP(I,1)              BO(I)
N                           0.56297811E-03        0.00000000E+00       0.56297811E-03
O                           0.36199557E-01        0.00000000E+00       0.36199557E-01
CL                          0.56297811E-03        0.00000000E+00       0.56297811E-03
C                           0.18286091E-01        0.00000000E+00       0.18286091E-01
H                           0.23621158E-01        0.00000000E+00       0.23621158E-01
K                           0.96679461E-02        0.00000000E+00       0.96679461E-02

POINT ITN    T        KCL            CO             HCL            CO2            H2O            H2
  1    20 3163.37  -42.372        -28.934         -30.674        -45.848        -34.315        -24.742
  2     6 2907.53  -43.186        -29.563         -31.489        -46.388        -35.258        -24.987
PC/PT= 1.758518    T =   2927.53
  2     3 2905.85  -43.192        -29.567         -31.414        -46.369        -35.257        -24.988
PC/PT= 1.765135    T =   2905.85
  2     2 2905.84  -43.192        -29.567         -31.414        -46.369        -35.257        -24.988
PC/PT= 1.765177    T =   2905.84
  3     7 1576.55  -51.603        -35.013         -38.586        -60.130        -44.632        -26.468
  3     3 1575.84  -51.621        -35.024         -38.608        -60.159        -44.651        -26.470
  4     5 1505.31  -52.515        -35.547         -39.330        -61.564        -45.684        -26.586
  4     3 1507.28  -52.491        -35.534         -39.311        -61.526        -45.579        -26.583
  5     6 1372.64  -54.526        -36.689         -40.948        -64.643        -47.594        -26.835
  5     3 1372.22  -54.533        -36.693         -40.954        -64.654        -47.702        -26.836
  6     5 1245.92  -56.954        -38.007         -42.862        -68.217        -50.122        -27.116
ADD KCL(L)
  6     3 1249.86  -56.959        -37.980         -42.849        -68.112        -50.056        -27.124
```

6	3	1251	37	-56 913	-37.961	-42.819	-68.863	-58.822	-27.118

THEORETICAL ROCKET PERFORMANCE ASSUMING EQUILIBRIUM COMPOSITION DURING EXPANSION

PC = 3000.0 PSIA
CASE NO. 208

	CHEMICAL FORMULA				WT FRACTION (SEE NOTE)	ENERGY CAL/MOL	STATE	TEMP DEG K
FUEL	K 1.00000	O 4.00000	CL 1.00000		0.878000	-103430.000	S	298.15
FUEL	C 6.00000	O 9.90000	H 7.55000	N 2.45000	0.546000	-169170.000	S	298.15
FUEL	C 3.00000	O 9.00000	H 5.00000	N 3.00000	0.355000	-88600.000	S	298.15
FUEL	C 17.00000	H 20.00000	O 1.00000	N 2.00000	0.009000	-25100.000	S	298.15
FUEL	C 1.00000				0.012000	0.000		0.00

O/F= 0.0000 PERCENT FUEL= 100.0000 EQUIVALENCE RATIO= 1.3540 PHI= 0.0000

	CHAMBER	THROAT	EXIT	EXIT	EXIT	EXIT
PC/P	1.0000	1.7652	63.857	82.035	140.42	244.52
P, ATM	340.23	192.74	5.3280	4.1474	2.4279	1.3914
T, DEG K	3163.4	2905.8	1575.0	1507.1	137 .2	1251.4
RHO, G/CC	3.6655-2	2.2697-2	1.1626-3	9.4615-4	6.0768-4	3.8360-4
H, CAL/G	-536.68	-658.89	-1212.76	-1239.95	-1294.38	-1345.44
U, CAL/G	-761.28	-864.54	-1323.74	-1346.10	-1390.94	-1433.28
G, CAL/G	-7393.34	-6957.33	-4626.68	-4506.57	-4268.70	-4057.80
S, CAL/(G)(K)	2.1675	2.1675	2.1675	2.1675	2.1675	2.1675
M, MOL WT	27.989	28.079	28.202	28.212	28.241	28.309
(DLV/DLP)T	-1.00371	-1.00189	-1.00081	-1.00098	-1.00129	-1.01123
(DLV/DLT)P	1.0748	1.0399	1.0115	1.0144	1.0207	1.1844
CP, CAL/(G)(K)	0.5282	0.4769	0.4039	0.4068	0.4153	0.6061
GAMMA (S)	1.1762	1.1885	1.2160	1.2154	1.2125	1.1782
SON VEL,M/SEC	1052.4	1011.2	751.4	734.7	699.9	658.8
MACH NUMBER	0.000	1.000	3.165	3.302	3.598	3.953

PERFORMANCE PARAMETERS

AE/AT	1.0000	8.3000	10.000	15.000	23.000
CSTAR, FT/SEC	4928	4928	4928	4928	4928
CF	0.673	1.584	1.615	1.677	1.732
IVAC,LB-SEC/LB	189.9	262.5	266.0	273.1	279.7
ISP, LB-SEC/LB	103.1	242.5	247.4	256.8	265.3

MOLE FRACTIONS

FORMALDEHYDE	2.7435-6	1.6194-6	9.1811-8	7.7084-8	5.3337-8	3.6505-8
FORMIC ACID	1.0412-5	5.7875-6	1.6383-7	1.2999-7	7.9736-8	4.8527-8
CH4	6.2423-9	4.4399-9	3.5754-8	5.5107-8	1.5707-7	5.0636-7
CO	2.9577-1	2.9229-1	2.5795-1	2.5360-1	2.4311-1	2.3079-1
COCL	2.351 -6	8.762 -7	5.242-11	2.841-11	2.351-12	2.126-13
CO2	2.1600-1	2.2113-1	2.5776-1	2.6229-1	2.7332-1	2.8608-1
CL	2.581 -4	1.325 -4	2.231 -8	8.734 -9	9.888-10	8.689-11
CLO	9.266 -7	2.156 -7	7.093-15	1.189-15	1.949-17	2.187-19
H	3.0335-3	1.8939-3	5.2374-6	2.8060-6	6.6799-7	1.4038-7
HCN	2.6045-6	1.5186-6	9.2577-8	7.8615-8	5.5888-8	3.9460-8
HCO RAD	4.008 -5	9.067 -6	8.326 -9	4.395 -9	1.039 -9	2.202-10
HCL	6.1897-3	5.2073-3	4.5892-4	3.4824-4	1.8022-4	8.1443-5
HNCO	2.3911-6	1.2876-6	2.6196-8	1.9905-8	1.1000-8	5.9332-9
HNO	2.315 -6	6.759 -7	1.932-12	5.701-13	3.348-14	1.574-15
HOCL	1.623 -6	5.363 -7	2.192-12	6.203-13	3.398-14	1.363-15
HO2	6.611 -6	1.339 -6	8.439-14	1.537-14	3.126-16	4.612-18
H2	4.9034-2	5.0971-2	8.5609-2	9.0087-2	1.0095-1	1.1357-1
H2O	2.7086-1	2.7318-1	2.4704-1	2.4278-1	2.3242-1	2.2018-1
H2O2	2.364 -6	6.811 -7	1.115-12	2.983-13	1.481-14	5.787-16
K	8.2420-4	7.3054-4	5.2514-5	3.7366-5	1.6481-5	6.0995-6

KCL	9.2315-3	1.0373-2	1.3356-2	1.2799-2	1.0928-2	7.7913-3
KH	3.0715-5	1.8597-5	8.5838-9	4.9147-8	1.3367-8	3.0826-9
KO	3.654 -5	1.430 -5	1.371-10	4.687-11	2.842-12	1.251-13
KOH	5.5599-3	4.5773-3	4.0628-4	3.1077-4	1.6377-4	7.5344-5
K2CL2	3.6550-5	4.6738-5	1.0318-3	1.3680-3	2.3958-3	3.2443-3
N	7.470 -7	1.958 -7	6.001-14	1.309-14	4.026-16	9.303-18
NH	2.303 -6	7.498 -7	6.907-12	2.207-12	1.648-13	9.893-15
NH2	2.308 -6	9.581 -7	4.077-10	2.004-10	4.631-11	7.194-12
NH3	3.7851-6	4.2663-6	2.5247-6	2.5729-6	2.7684-6	3.0523-6
NO	1.186 -3	4.811 -4	9.673 -9	3.139 -9	2.411-10	1.494-11
NO2	5.731 -7	1.146 -7	1.291-15	2.019-16	2.917-18	2.993-20
N2	1.3469-1	1.3548-1	1.3633-1	1.3638-1	1.3652-1	1.3663-1
N2O	5.218 -7	1.574 -7	5.594-13	1.641-13	1.018-14	5.831-16
O	2.367 -4	7.273 -5	2.815-11	5.948-12	1.667-13	3.458-15
OH	6.4368-3	3.2034-3	5.6485-7	2.2748-7	2.0217-8	2.9224-9
O2	5.191 -4	1.567 -4	3.727-11	7.444-12	1.842-13	3.325-15
KCL(L)	0.0000 0	0.0000 0	0.0000 0	0.0000 0	0.0000 0	1.5516-3

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.50000E-06 FOR ALL ASSIGNED CONDITIONS

C	CCL	CCL2	CCL3	CCL4	CH	CHCL
CHCL3	CH2	CH2CL2	CH3	CH3CL	HYDROXYMETHYLENE	METHYLOXIDE
METHANOL	CN	HCN RAD	CHN RAD	COCL2	C2	C2CL2
C2CL4	C2CL6	C2H RAD	C2HCL	ACETYLENE	KETENE	C2H3 RAD
METHYL CYANIDE	CH3CO RAD	CH2CHO RAD	ETHYLENE	ACETALDEHYDE	ACETIC ACID	(FORMIC ACID)2
ETHYL RAD	ETHYL OXIDE RAD	ETHANE	AZOMETHANE	DIMETHYL ETHER	ETHANOL	CNC RAD
CYANOGEN	CCO RAD	C3	C3H3 RAD	CYCLOPROPENE	PROPYNE	ALLENE
C3H5 RAD	CYCLOPROPANE	PROPYLENE	PROPYLENE OXIDE	I-PROPYL RAD	N-PROPYL RAD	PROPANE
1-PROPANOL	CARBON SUBOXIDE	C4	BUTADIYNE	CYCLOBUTADIENE	BUTAN-1EN-3YN	1,3-BUTADIENE
2-BUTYNE	2-BUTENE TRANS	2-BUTENE CIS	ISOBUTENE	1-BUTENE	(ACETIC ACID)2	T-BUTYL RAD
S-BUTYL RAD	N-BUTYL RAD	N-BUTANE	ISOBUTANE	CARBON SUBNITRID	C5	CYCLOPENTADIENE
CYCLOPENTANE	1-PENTENE	T-PENTYL RAD	N-PENTYL RAD	PENTANE	ISOPENTANE	CH3C(CH3)2CH3
HEXATRIYNE	PHENYL RAD	PHENOXY RAD	BENZENE	PHENOL	CYCLOHEXENE	N-HEXYL RAD
TOLUENE	CRESOL	1-HEPTENE	N-HEPTYL RAD	N-HEPTANE	1-OCTENE	N-OCTYL RAD
OCTANE	ISO-OCTANE	N-NONYL RAD	NAPTHLENE	AZULENE	N-DECYL RAD	O-BIPHENYL RAD
BIPHENYL	JET-A(G)	CLCN	CLO2	CL2	CL2O	HNO2
HNO3	N2H2	KCN	K2	K2C2N2	K2O2H2	NCO
NH2OH	NOCL	NO2CL	NO3	N2H2	NH2NO2	N2H4
N2O3	N2O4	N2O5	N3	N3H	O3	C(GR)
BENZENE(L)	TOLUENE(L)	OCTANE(L)	JET-A(L)	H2O(S)	H2O(L)	K(S)
K(L)	KCN(S)	KCN(L)	KCL(S)	KOH(A)	KOH(B)	KOH(L)
KO2(S)	K2CO3(S)	K2CO3(L)	K2O(S)	K2O2(S)	NH4CL(A)	NH4CL(B)

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

THEORETICAL ROCKET PERFORMANCE ASSUMING FROZEN COMPOSITION DURING EXPANSION

PC = 5000.0 PSIA
CASE NO. 208

	CHEMICAL FORMULA				WT FRACTION (SEE NOTE)	ENERGY CAL/MOL	STATE	TEMP DEG K
FUEL	K 1.00000	O 4.00000	CL 1.00000		0.079800	-103430.000	S	298.15
FUEL	C 6.00000	O 9.90000	H 7.55000	N 2.45000	0.546000	-169170.000	S	298.15
FUEL	C 3.00000	O 9.00000	H 5.00000	N 3.00000	0.355000	-88600.000	S	298.15
FUEL	C 17.00000	H 20.00000	O 1.00000	N 2.00000	0.009600	-25100.000	S	298.15
FUEL	C 1.00000				0.012000	0.000		0.00

O/F= 0.0000 PERCENT FUEL= 100.0000 EQUIVALENCE RATIO= 1.3540 PHI= 0.0000

	CHAMBER	THROAT	EXIT	EXIT	EXIT	EXIT
PC/P	1.0000	1.7792	66.410	85.697	148.53	263.93
P, ATM	340.73	191.23	5.1231	3.9701	2.2906	1.2891
T, DEG K	3163.4	2561.2	1477.4	1406.5	1262.1	1124.3
RHO, G/CC	3.6685-2	2.2797-2	1.1828-3	9.6795-4	6.1984-4	3.9111-4
H, CAL/G	-536.68	-659.81	-1200.66	-1226.76	-1278.82	-1327.48
U, CAL/G	-761.78	-862.95	-1305.56	-1326.61	-1368.43	-1407.30
G, CAL/G	-7393.34	-6861.46	-4403.04	-4274.90	-4014.49	-3764.33
S, CAL/(G)(K)	2.1675	2.1675	2.1675	2.1675	2.1675	2.1675
M, MOL WT	27.989	27.989	27.989	27.989	27.989	27.989
CP, CAL/(G)(K)	0.4092	0.4055	0.3685	0.3650	0.3571	0.3485
GAMMA (S)	1.2099	1.2122	1.2387	1.2415	1.2482	1.2558
SON VEL,M/SEC	1066.3	1015.1	737.3	720.2	684.1	647.6
MACH NUMBER	0.000	1.000	3.197	3.337	3.643	3.972

PERFORMANCE PARAMETERS

AE/AT	1.0000	8.3000	10.000	15.000	23.000
CSTAR, FT/SEC	4888	4888	4888	4888	4888
CF	0.681	1.582	1.613	1.673	1.727
IVAC,LB-SEC/LB	188.9	259.4	262.8	269.5	275.6
ISP, LB-SEC/LB	103.5	240.4	245.8	254.1	262.3

MOLE FRACTIONS

FORMALDEHYDE	0.00000	FORMIC ACID	0.00001	CO	0.29577	COCL	0.00000
CO2	0.21600	CL	0.00026	CLO	0.00083	H	0.00303
HCN	0.00000	HCO RAD	0.00002	HCL	0.00619	HNCO	0.00000
HNO	0.00000	HOCL	0.00000	HO2	0.00001	H2	0.04903
H2O	0.27086	H2O2	0.00000	K	0.00082	KCL	0.00923
KH	0.00003	KO	0.00004	KOH	0.06556	K2CL2	0.00004
N	0.00000	NH	0.00000	NH2	0.00000	NH3	0.00001
NO	0.00119	NO2	0.00000	N2	0.13469	N2O	0.00000
O	0.00024	OH	0.00644	O2	0.00052		

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.50000E-06 FOR ALL ASSIGNED CONDITIONS

C	CCL	CCL2	CCL3	CCL4	CH	CHCL
CHCL3	CH2	CH2CL2	CH3	CH3CL	HYDROXYMETHYLENE	METHYLOXIDE
CH4	METHANOL	CN	NCN RAD	CNN RAD	COCL2	C2
C2CL2	C2CL4	C2CL6	C2H RAD	C2HCL	ACETYLENE	KETENE
C2H3 RAD	METHYL CYANIDE	CH3CO RAD	CH2CHO RAD	ETHYLENE	ACETALDEHYDE	ACETIC ACID
(FORMIC ACID)2	ETHYL RAD	ETHYL OXIDE RAD	ETHANE	AZOMETHANE	DIMETHYL ETHER	ETHANOL
CNC RAD	CYANOGEN	CCO RAD	C3	C3H3 RAD	CYCLOPROPENE	PROPYNE
ALLENE	C3H5 RAD	CYCLOPROPANE	PROPYLENE	PROPYLENE OXIDE	I-PROPYL RAD	N-PROPYL RAD
PROPANE	1-PROPANOL	CARBON SUBOXIDE	C4	BUTADIYNE	CYCLOBUTADIENE	BUTAN-1EN-3YN
1,3-BUTADIENE	2-BUTYNE	2-BUTENE TRANS	2-BUTENE CIS	ISOBUTENE	1-BUTENE	(ACETIC ACID)2
T-BUTYL RAD	S-BUTYL RAD	N-BUTYL RAD	N-BUTANE	ISOBUTANE	CARBON SUBNITRID	C5

CYCLOPENTADIENE	CYCLOPENTANE	1-PENTENE	T-PENTYL RAD	N-PENTYL RAD	PENTANE	ISOPENTANE
CH3C(CH3)2CH3	HEXATRIYNE	PHENYL RAD	PHENOXY RAD	BENZENE	PHENOL	CYCLOHEXENE
N-HEXYL RAD	TOLUENE	CRESOL	1-HEPTENE	N-HEPTYL RAD	N-HEPTANE	1-OCTENE
N-OCTYL RAD	OCTANE	ISO-OCTANE	N-NONYL RAD	NAPTHLENE	AZULENE	N-DECYL RAD
O-BIPHENYL RAD	BIPHENYL	JET-A(G)	CLCN	CLO2	CL2	CL2O
HNO2	HNO3	N2H2	KCN	K2	K2C2N2	K2O2H2
HCO	NH2OH	NOCL	NO2CL	NO3	N2H2	NH2NO2
N2H4	N2O3	N2O4	N2O5	N3	N3H	O3
C(GR)	BENZENE(L)	TOLUENE(L)	OCTANE(L)	JET-A(L)	H2O(S)	H2O(L)
K(S)	K(L)	KCN(S)	KCN(L)	KCL(S)	KCL(L)	KOH(A)
KOH(B)	KOH(L)	KO2(S)	K2CO3(S)	K2CO3(L)	K2O(S)	K2O2(S)
NH4CL(A)	NH4CL(B)					

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

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REACTANTS
K    1.0000  C    4.0000  CL   1.0000          0.0000       0.0000    0.050000    -103430.00  S    298.150     F
C    6.0000  O    9.0000  H    7.5500  N    2.4500       0.0000   54.599998    -169170.00  S    298.150     F
C    3.0000  O    9.0000  H    5.0000  N    3.0000       0.0000   35.500000     -88600.00  S    298.150     F
C   17.0000  H   28.0000  O    1.0000  N    2.0000       0.0000    8.900000     -25100.00  S    298.150     F
C    1.0000       0.0000       0.0000       0.0000       0.0000    1.200000          0.00          0.000

NAMELISTS
$INPT2
KASE     =          208.
T        = 26*0.00000000E+00,
P        =    5000.000      , 25*0.00000000E+00,
PSIA     = T,
NMHG     = F,
NSQM     = F,
V        = 26*0.00000000E+00,
RHO      =    5000.000      , 25*0.00000000E+00,
ERATIO   = F,
OF       = F,
FPCT     = F,
FA       = F,
MIX      = 26*-1.000000      ,
TP       = F,
HP       = F,
SP       = F,
TV       = F,
UV       = F,
SV       = F,
RKT      = T,
SHOCK    = F,
DETN     = F,
TRACE    =  5.0000000000000000E-07,
SO       =  0.0000000000000000E+00,
SO       =  0.00000000E+00,
IONS     = F,
IDEBUG   =           0,
PHI      = F,
SIUNIT   = F,
INHG     = F,
TRNSPT   = F,
TRPACC   =  0.99990000000000000      ,
DIF      = F,
NODATA   = F,
U        =  1.0000000000000000E+30,
H        =  1.0000000000000000E+30
$END

NO INPT2 VALUE GIVEN FOR OF, EQRAT, FA, OR FPCT
$RKTINP
EQL      = T,
FROZ     = T,
SUBAR    = 13*0.0000000000000000E+00,
SUPAR    =    0.30000000000000000      ,    10.000000000000000      ,
  15.000000000000000      ,    23.000000000000000      , 9*0.0000000000000000E+00,
PCP      = 22*0.0000000000000000E+00,
TCEST    =    3800.000      ,
NFZ      =           1
$END

OF =    0.000000
                              EFFECTIVE FUEL          EFFECTIVE OXIDANT            MIXTURE
ENTHALPY                          HPP(2)                  HPP(1)                    HSUB0
(KG-MOL)(DEG K)/KG          -0.27833260E+03          0.00000000E+00          -0.27833260E+03
```

KG-FRMN.WT./KG	BOP(I,2)	BOP(I,1)	BO(I)
K	0.57957348E-03	0.00000000E+00	0.57957348E-03
O	0.36181282E-01	0.00000000E+00	0.36181282E-01
CL	0.57957348E-03	0.00000000E+00	0.57957348E-03
C	0.10240491E-01	0.00000000E+00	0.10240491E-01
H	0.23562253E-01	0.00000000E+00	0.23562253E-01
N	0.96438378E-02	0.00000000E+00	0.96438378E-02

POINT	ITN	T	KCL	CO	HCL	CO2	H2O	N2
1	20	3166.98	-42.330	-26.939	-30.653	-45.025	-34.310	-24.747
2	6	2911.78	-43.144	-29.567	-31.387	-46.359	-35.242	-24.993
PC/PT= 1.758159			T = 2911.78					
2	3	2918.09	-43.150	-29.571	-31.392	-46.368	-35.249	-24.994
PC/PT= 1.764784			T = 2918.09					
2	2	2918.08	-43.150	-29.571	-31.392	-46.369	-35.249	-24.994
PC/PT= 1.764826			T = 2918.08					
3	7	1580.66	-51.538	-35.004	-38.543	-60.061	-44.590	-26.476
3	3	1579.26	-51.554	-35.014	-38.557	-60.087	-44.608	-26.478
4	5	1509.55	-52.444	-35.535	-39.283	-61.485	-45.556	-26.594
4	3	1511.21	-52.421	-35.522	-39.265	-61.450	-45.532	-26.591
5	6	1376.50	-54.448	-36.674	-40.896	-64.556	-47.641	-26.843
5	3	1376.18	-54.454	-36.677	-40.901	-64.565	-47.646	-26.843
6	6	1249.79	-56.041	-37.986	-42.799	-68.189	-50.053	-27.123
ADD KCL(L)								
6	3	1253.40	-56.863	-37.961	-42.786	-68.014	-49.994	-27.131
6	3	1254.79	-56.826	-37.543	-42.758	-67.965	-49.963	-27.126

THEORETICAL ROCKET PERFORMANCE ASSUMING EQUILIBRIUM COMPOSITION DURING EXPANSION

PC = 5000 0 PSIA
CASE NO. 200

	CHEMICAL FORMULA				WT FRACTION (SEE NOTE)	ENERGY CAL/MOL	STATE	TEMP DEG K
FUEL	K 1.00000	O 4.00000	CL 1.00000		0.080299	-103430.000	S	298.15
FUEL	C 6.00000	O 9.90000	H 7.55000	N 2.45000	0.544638	-169170.000	S	298.15
FUEL	C 3.00000	O 9.00000	H 5.00000	N 3.00000	0.354115	-88600.000	S	298.15
FUEL	C 17.00000	H 20.00000	O 1.00000	N 2.00000	0.008978	-25180.000	S	298.15
FUEL	C 1.00000				0.011970	0.000		0.00

O/F= 0 0000 PERCENT FUEL= 100.0000 EQUIVALENCE RATIO= 1.3312 PHI= 0.0000

	CHAMBER	THROAT	EXIT	EXIT	EXIT	EXIT
PC/P	1.0000	1 7648	63.795	81.952	140.27	244.29
P, ATM	340.23	192.78	5 3331	4.1516	2.4255	1.3927
T, DEG K	3167.8	2910.1	1579.3	1511.2	1376.2	1254.8
RHO, G/CC	3.6712-2	2.2712-2	1.1630-3	9.4643-4	6.0785-4	3.8369-4
H, CAL/G	-537.20	-659.29	-1213.11	-1240.31	-1294.78	-1345.09
U, CAL/G	-761 64	-824.05	-1324.16	-1346.34	-1391.42	-1433.80
G, CAL/G	-7394.79	-6960.62	-4632.74	-4512.60	-4274.67	-4062.95
S, CAL/(G)(K)	2.1653	2.1653	2.1653	2.1653	2.1653	2.1653
M, MOL WT	28.041	28.132	28 259	28.269	28.299	28.366
(DLV/DLP)T	-1.00379	-1.00194	-1.00003	-1.00101	-1.00133	-1.01173
(DLV/DLT)P	1.0764	1.0400	1.0110	1.0140	1.0213	1.1921
CP, CAL/(G)(K)	0.52[illegible]	0 4779	0.4038	0.4066	0.4152	0.6131
GAMMA (S)	1.1781	1 1879	1.2157	1.2151	1.2122	1.1773
SON VEL,M/SEC	1051 [illegible]	1010.0	751 6	734.9	700.1	650.0
MACH NUMBER	0.000	1.000	3.164	3.301	3.596	3.953

PERFORMANCE PARAMETERS

AE/AT	1.0000	8.3000	10.000	15.000	25.000
CSTAR, FT/SEC	4927	4927	4927	4927	4927
CF	0 673	1.584	1.615	1.677	1.732
IVAC,LB-SEC/LB	189.0	262 4	266.0	273.1	279.7
ISP, LB-SEC/LB	103.1	242.5	247.3	256.7	265.3

MOLE FRACTIONS

FORMALDEHYDE	2.6993-6	1.5921-6	9.0204-8	7.5734-8	5.2482-8	3.5878-8
FORMIC ACID	2.0364-5	5.7635-6	1.6323-7	1 2951-7	7.9439-8	4.8342-8
CO	2.9422-1	2.9072-1	2.5572-1	2.5242-1	2.4284-1	2.2982-1
COCL	2.418 -6	9.041 -7	5.583-11	2.182-11	2.534-12	2.389-13
CO2	2.1722-1	2.2241-1	2.5874-1	2.6323-1	2.7416-1	2.8686-1
CL	2.678 -4	1.381 -4	2.423 -8	9.526 -9	1.890 -9	9.569-11
CLO	9.021 -7	2.304 -7	8.185-15	1.383-15	2.389-17	2.524-19
H	3 0467-3	1 9691-3	5.4497-6	2.9290-6	7.8245-7	1.4082-7
HCN	[illegible]	1.4834-6	9.8296-8	7.6672-8	5.4495-8	3.8402-8
HCO RAD	[illegible]	[illegible]	8.502 -9	4.498 -9	1.869 -9	2.278-10
HCL	6.3228-3	5.3228-3	4.7386-4	3.6607-4	1.8793-4	8.5038-5
HNCO	2 3663-6	1 2745-6	2.5993-8	1.9756-8	1.0924-8	5.8936-9
HNO	2.365 -6	6 952 -7	2.147-12	6.288-13	3.698-14	1.741-15
HOCL	1 697 -6	5.641 -7	2.425-12	6.900-13	3.829-14	1.550-15
HO2	6.879 -6	1 617 -6	9.560-14	1.754-14	3.631-16	5.300-18
H2	4 0488-2	5 0387-2	8.4639-2	8.9072-2	9.9829-2	1.1237-1
H2O	2.7100-1	2.7341-1	2.4783-1	2.4363-1	2.3339-1	2.2125-1
H2O2	2 431 -6	7 055 -7	1.221-12	3.285-13	1.652-14	6.484-16
K	8.4006-4	7 4531-4	5.4454-5	3.8829-5	1.7137-5	6.4173-6
KCL	9.5778-3	1 0743-2	1.3785-2	1.3216-2	1.1307-2	8.1459-3

KH	3.1177-5	1.8986-5	8.9166-8	5.1188-8	1.4816-8	3.1716-9
KO	3.807 -5	1.499 -5	1.734-10	5.280-11	3.197-12	1.428-13
KOH	5.6854-3	4.6827-3	4.1927-4	3.2213-4	1.6983-4	7.8621-5
K2CL2	3.9853-5	4.9623-5	1.0598-3	1.4848-3	2.4537-3	3.3843-3
N	7.625 -7	2.815 -7	6.612-14	1.452-14	4.537-16	1.654-17
NH	2.525 -6	7.607 -7	7.557-12	2.362-12	1.776-13	1.875-14
NH2	2.293 -6	9.577 -7	4.187-10	2.263-10	4.177-11	7.474-12
NH3	8.6178-6	6.1392-6	2.4555-6	2.5808-6	2.6865-6	2.9625-6
NO	1.217 -3	4.971 -4	1.846 -8	3.438 -9	2.665-10	1.658-11
NO2	6.884 -7	1.215 -7	1.481-15	2.336-16	3.438-18	3.548-20
N2	1.3459-1	1.3540-1	1.3626-1	1.3631-1	1.3646-1	1.3658-1
N2O	5.356 -7	1.626 -7	6.877-13	1.791-13	1.116-14	5.574-16
O	2.448 -4	7.592 -5	3.163-11	6.723-12	1.920-13	3.994-15
OH	6.5574-3	3.2810-3	6.8521-7	2.4423-7	3.8614-8	3.1817-9
O2	5.432 -4	1.656 -4	4.246-11	8.544-12	2.151-13	3.905-15
KCL(L)	0.0000 0	0.0000 0	0.0000 0	0.0000 0	0.0000 0	1.4174-3

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.50000E-05 FOR ALL ASSIGNED CONDITIONS

C	CCL	CCL2	CCL3	CCL4	CH	CHCL
CHCL3	CH2	CH2CL2	CH3	CH3CL	HYDROXYMETHYLENE	METHYLOXIDE
CH4	METHANOL	CN	HCN RAD	CNN RAD	COCL2	C2
C2CL2	C2CL4	C2CL6	C2H RAD	C2HCL	ACETYLENE	KETENE
C2H3 RAD	METHYL CYANIDE	CH3CO RAD	CH2CHO RAD	ETHYLENE	ACETALDEHYDE	ACETIC ACID
(FORMIC ACID)2	ETHYL RAD	ETHYL OXIDE RAD	ETHANE	AZOMETHANE	DIMETHYL ETHER	ETHANOL
CNC RAD	CYANOGEN	CCO RAD	C3	C3H3 RAD	CYCLOPROPENE	PROPYNE
ALLENE	C3H5 RAD	CYCLOPROPANE	PROPYLENE	PROPYLENE OXIDE	I-PROPYL RAD	N-PROPYL RAD
PROPANE	1-PROPANOL	CARBON SUBOXIDE	C4	BUTADIYNE	CYCLOBUTADIENE	BUTAN-1EN-3YN
1,3-BUTADIENE	2-BUTYNE	2-BUTENE TRANS	2-BUTENE CIS	ISOBUTENE	1-BUTENE	(ACETIC ACID)2
T-BUTYL RAD	S-BUTYL RAD	N-BUTYL RAD	N-BUTANE	ISOBUTANE	CARBON SUBNITRID	C5
CYCLOPENTADIENE	CYCLOPENTANE	1-PENTENE	T-PENTYL RAD	N-PENTYL RAD	PENTANE	ISOPENTANE
CH3C(CH3)2CH3	HEXATRIYNE	PHENYL RAD	PHENOXY RAD	BENZENE	PHENOL	CYCLOHEXENE
N-HEXYL RAD	TOLUENE	CRESOL	1-HEPTENE	N-HEPTYL RAD	N-HEPTANE	1-OCTENE
N-OCTYL RAD	OCTANE	ISO-OCTANE	N-NONYL RAD	NAPTHLENE	AZULENE	N-DECYL RAD
O-BIPHENYL RAD	BIPHENYL	JET-A(G)	CLCN	CLO2	CL2	CL2O
HNO2	HNO3	H2N2	HCN	K2	K2C2N2	K2O2H2
NCO	NH2OH	NOCL	NO2CL	NO3	N2H2	NH2NO2
N2H4	N2O3	N2O4	N2O5	N3	N3H	O3
C(GR)	BENZENE(L)	TOLUENE(L)	OCTANE(L)	JET-A(L)	H2O(S)	H2O(L)
K(S)	K(L)	KCN(S)	KCN(L)	KCL(S)	KOH(A)	KOH(B)
KOH(L)	KO2(S)	K2CO3(S)	K2CO3(L)	K2O(S)	K2O2(S)	NH4CL(A)
NH4CL(B)						

NOTE WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

THEORETICAL ROCKET PERFORMANCE ASSUMING FROZEN COMPOSITION DURING EXPANSION

PC = 5500.0 PSIA
CASE NO. 280

	CHEMICAL FORMULA				WT FRACTION (SEE NOTE)	ENERGY CAL/MOL	STATE	TEMP DEG K
FUEL	K 1.00000	O 4.00000	CL 1.00000		0.080299	-103430.000	S	298.15
FUEL	C 6.00000	O 9.90000	H 7.55000	N 2.45000	0.544638	-169170.000	S	298.15
FUEL	C 3.00000	O 9.00000	H 5.00000	N 3.00000	0.354115	-88600.000	S	298.15
FUEL	C 17.00000	H 20.00000	O 1.00000	N 2.00000	0.008978	-25100.000	S	298.15
FUEL	C 1.00000				0.011970	0.000		0.00

O/F= 0.0000 PERCENT FUEL= 100.0000 EQUIVALENCE RATIO= 1.3312 PHI= 0.0000

	CHAMBER	THROAT	EXIT	EXIT	EXIT	EXIT
PC/P	1.0000	1.7790	66.361	85.629	148.39	263.63
P, ATM	380.23	191.74	5.1269	3.9733	2.2928	1.2905
T, DEG K	3167.0	2864.7	1488.5	1409.2	1265.0	1127.0
RHO, G/CC	3.6712-2	2.2813-2	1.1134-3	9.6348-4	6.1937-4	3.9131-4
H, CAL/G	-537.28	-650.23	-1208.03	-1226.93	-1278.99	-1327.66
U, CAL/G	-761.64	-863.25	-1305.75	-1326.89	-1368.64	-1407.53
G, CAL/G	-7394.79	-6863.34	-4486.52	-4278.43	-4018.13	-3768.04
S, CAL/(G)(K)	2.1653	2.1653	2.1653	2.1653	2.1653	2.1653
M, MOL WT	28.541	28.841	28.841	28.841	28.841	28.841
CP, CAL/(G)(K)	0.4088	0.4051	0.3682	0.3647	0.3569	0.3484
GAMMA (S)	1.2697	1.2120	1.2383	1.2412	1.2478	1.2553
SON VEL, M/SEC	1065.8	1014.6	737.3	720.2	684.1	647.7
MACH NUMBER	0.000	1.000	3.196	3.336	3.642	3.971

PERFORMANCE PARAMETERS

AE/AT	1.0000	8.3000	10.000	15.000	23.000
CSTAR, FT/SEC	4886	4886	4886	4886	4886
CF	0.681	1.582	1.613	1.673	1.727
IVAC, LB-SEC/LB	188.8	259.3	262.7	269.4	275.5
ISP, LB-SEC/LB	183.5	248.3	245.0	254.1	262.3

MOLE FRACTIONS

FORMALDEHYDE	0.00000	FORMIC ACID	0.00001	CO	0.29422	COCL	0.00000
CO2	0.21722	CL	0.00027	CL2	0.00000	H	0.00305
HCN	0.00000	HCO RAD	0.00002	HCL	0.08632	HNCO	0.00000
HNO	0.00000	HOCL	0.00000	HO2	0.00001	H2	0.04849
H2O	0.27100	H2O2	0.00000	K	0.06084	KCL	0.00958
KH	0.00003	KO	0.00004	KOH	0.00569	K2CL2	0.00004
N	0.00000	NH	0.00000	NH2	0.00000	NH3	0.00001
NO	0.00122	NO2	0.00000	N2	0.13459	N2O	0.00000
O	0.00024	OH	0.00656	O2	0.00054		

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.50000E-06 FOR ALL ASSIGNED CONDITIONS

C	CCL	CCL2	CCL3	CCL4	CH	CHCL
CHCL3	CH2	CH2CL2	CH3	CH3CL	HYDROXYMETHYLENE	METHYLOXIDE
CH4	METHANOL	CN	NCN RAD	CNN RAD	COCL2	C2
C2CL2	C2CL4	C2CL6	C2H RAD	C2HCL	ACETYLENE	KETENE
C2H3 RAD	METHYL CYANIDE	CH3CO RAD	CH2CHO RAD	ETHYLENE	ACETALDEHYDE	ACETIC ACID
(FORMIC ACID)2	ETHYL RAD	ETHYL OXIDE RAD	ETHANE	AZOMETHANE	DIMETHYL ETHER	ETHANOL
CNC RAD	CYANOGEN	CCO RAD	C3	C3H3 RAD	CYCLOPROPENE	PROPYNE
ALLENE	C3H5 RAD	CYCLOPROPANE	PROPYLENE	PROPYLENE OXIDE	I-PROPYL RAD	N-PROPYL RAD
PROPANE	1-PROPANOL	CARBON SUBOXIDE	C4	BUTADIYNE	CYCLOBUTADIENE	BUTAN-1EN-3YN
1,3-BUTADIENE	2-BUTYNE	2-BUTENE TRANS	2-BUTENE CIS	ISOBUTENE	1-BUTENE	(ACETIC ACID)2
T-BUTYL RAD	S-BUTYL RAD	N-BUTYL RAD	N-BUTANE	ISOBUTANE	CARBON SUBNITRID	C5

CYCLOPENTADIENE	CYCLOPENTANE	1-PENTENE	T-PENTYL RAD	N-PENTYL RAD	PENTANE	ISOPENTANE
CH3C(CH3)2CH3	HEXATRIYNE	PHENYL RAD	PHENOXY RAD	BENZENE	PHENOL	CYCLOHEXENE
N-HEXYL RAD	TOLUENE	CRESOL	1-HEPTENE	N-HEPTYL RAD	N-HEPTANE	1-OCTENE
N-OCTYL RAD	OCTANE	ISO-OCTANE	N-NONYL RAD	NAPTHLENE	AZULENE	N-DECYL RAD
O-BIPHENYL RAD	BIPHENYL	JET-A(G)	CLCN	CLO2	CL2	CL2O
HNO2	HNO3	N2H2	KCN	K2	K2C2N2	K2O2H2
NCO	NH2OH	NOCL	NO2CL	NO3	N2H2	NH2NO2
N2H4	N2O3	N2O4	N2O5	N3	N3H	O3
C(GR)	BENZENE(L)	TOLUENE(L)	OCTANE(L)	JET-A(L)	H2O(S)	H2O(L)
K(S)	K(L)	KCN(S)	KCN(L)	KCL(S)	KCL(L)	KOH(A)
KOH(B)	KOH(L)	KO2(S)	K2CO3(S)	K2CO3(L)	K2O(S)	K2O2(S)
NH4CL(A)	NH4CL(B)					

NOTE WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

Table C-3

NASA - Lewis CET - 86

Output

Composition L

Tue Dec 3 10:16:43 EDT 1991

CWN

COMPL2.LAS

```
REACTANTS
N   1.0000  O   4.0000  N    4.0000  CL  1.0000      0.0000  73.930000    -78580.00  S    298.150   F
C   2.0000  CL  1.0000  N    3.0000      0.0000      0.0390  11.670000      9488.00  S    298.150   F
C  22.0000  O   4.0000  N   42.0000      0.0000      0.0000  11.670000   -308000.00  S    298.150   F
C   1.0000      0.0000       0.0000      0.0000      0.0000   0.850000         0.00         0.000
AL  1.0000      0.0000       0.0000      0.0000      0.0000   0.990000         0.00         0.000
BA  1.0000  CO  1.0000       0.0000      0.0000      0.0000   0.470000         0.00         0.000
CU  2.0000  CR  2.0000  O    4.0000      0.0000      0.0000   0.970000         0.00         0.000

NAMELISTS
SINPT2
KASE     =          208.
T        = 26*0.0000000E+00,
P        =    2500.000     , 25*0.0000000E+00,
PSIA     = T,
NMHG     = F,
NSQM     = F,
V        = 26*0.0000000E+00,
RHO      =    2500.000     , 25*0.0000000E+00,
ERATIO   = F,
OF       = F,
FPCT     = F,
FA       = F,
MIX      = 26*-1.000000    ,
TP       = F,
HP       = F,
SP       = F,
TV       = F,
UV       = F,
SV       = F,
RKT      = T,
SHOCK    = F,
DETN     = F,
TRACE    =  5.0000000000000000E-07,
S0       =  0.0000000000000000E+00,
S0       =  0.0000000E+00,
IONS     = F,
IDEBUG   =          L,
PHI      = F,
SIUNIT   = F,
INHG     = F,
TRNSPT   = F,
TRPACC   =  0.9999000000000000    ,
DIF      = F,
NODATA   = F,
U        =  1.0000000000000000E+30,
H        =  1.0000000000000000E+30
$END

NO INPT2 VALUE GIVEN FOR OF, EQRAT, FA, OR FPCT

SPECIES BEING CONSIDERED IN THIS SYSTEM
 J 6/79  AL                 J 6/63  ALC             J 9/79  ALCL            J 6/76  ALCL2           J 9/79  ALCL3
 J 6/63  ALH                J12/79  ALN             J12/79  ALO             J 9/64  ALOCL           J12/67  ALOH
 J12/79  ALO2               J12/68  ALO2H           J 6/79  AL2             J 9/79  AL2CL6          J12/79  AL2O
 J12/79  AL2O2              J12/70  BA              J12/72  BACL            J12/72  BACL2           J12/75  BAOH
 J12/75  BAO2H2             J 3/78  C               J12/69  CCL             J12/68  CCL2            J 6/70  CCL3
 P12/81  CCL4               J12/67  CH              RUS 79  CHCL            P 6/81  CHCL3           J12/72  C
 P12/81  CH2CL2             J 3/61  FORMALDEHYDE    L 4/85  FORMIC ACID     J 6/69  CH3             P12/81  CH...
 L 9/85  HYDROXYMETHYLENE   L 9/85  METHYLOXIDE     L 5/84  CH4             L 9/85  METHANOL        J 6/69  CN
 J12/70  HCN RAD            J 6/66  CNN RAD         J 9/65  CO              J12/65  COCL            J 6/61  COCL
 J 9/65  CO2                J12/69  C2              J12/68  C2CL2           L10/87  C2CL4           L10/87
 J 3/67  C2H RAD            RUS 79  C2HCL           J 3/61  ACETYLENE       BUR 84  KETENE          BUR 84     .3 RAD
 BUR 84  METHYL CYANIDE     BUR 84  CH3CO RAD       BUR 84  CH2CHO RAD      L 4/85  ETHYLENE        BUR 84  ACETALDEHYDE
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 L 4/85  ACETIC ACID          L 4/85  (FORMIC ACID)2       P10/85  ETHYL RAD            BUR 84  ETHYL OXIDE RAD      L 5/84  ETHANE
 BUR 84  AZOMETHANE           BUR 84  DIMETHYL ETHER       BUR 84  ETHANOL              J 3/67  CHC RAD              J 3/61  CYANOGEN
 J 9/66  CCO RAD              J12/69  C3                   D86/61  C3H3 RAD             BUR 84  CYCLOPROPENE         BUR 84  PROPYNE
 BUR 84  ALLENE               BUR 84  C3H5 RAD             BUR 84  CYCLOPROPANE         L 4/85  PROPYLENE            L 9/85  PROPYLENE OXIDE
 L 9/85  I-PROPYL RAD         L 9/85  N-PROPYL RAD         L 4/85  PROPANE              L 1/84  1-PROPANOL           J 6/68  CARBON SUBOXIDE
 J12/69  C4                   BUR 84  BUTADIYNE            P10/85  CYCLOBUTADIENE       BUR 84  BUTAN-1EN-3YN        P 4/84  1,3-BUTADIENE
 BUR 84  2-BUTYNE             BUR 84  2-BUTENE TRANS       BUR 84  2-BUTENE CIS         BUR 84  ISOBUTENE            BUR 84  1-BUTENE
 L 4/85  (ACETIC ACID)2       L 9/85  T-BUTYL RAD          L 9/85  S-BUTYL RAD          P10/83  N-BUTYL RAD          L 4/85  N-BUTANE
 L 4/85  ISOBUTANE            J 3/61  CARBON SUBNITRID     J12/69  C5                   P10/85  CYCLOPENTADIENE      P12/52  CYCLOPENTANE
 P12/52  1-PENTENE            L 5/87  T-PENTYL RAD         P10/83  N-PENTYL RAD         P10/85  PENTANE              P10/85  ISOPENTANE
 P10/85  CH3C(CH3)2CH3        BUR 84  HEXATRIYNE           L12/84  PHENYL RAD           L12/84  PHENOXY RAD          L12/84  BENZENE
 L12/84  PHENOL               BUR 84  CYCLOHEXENE          P10/83  N-HEXYL RAD          P10/84  TOLUENE              L 6/87  CRESOL
 P12/52  1-HEPTENE            P10/83  N-HEPTYL RAD         P 4/81  N-HEPTANE            P12/52  1-OCTENE             P10/83  N-OCTYL RAD
 P 4/85  OCTANE               P 4/85  ISO-OCTANE           P10/83  N-NONYL RAD          BUR 84  NAPTHLENE            BUR 84  AZULENE
 P10/83  N-DECYL RAD          L12/84  O-BIPHENYL RAD       L12/84  BIPHENYL             L 6/88  JET-A(G)             J 6/72  CL
 J 6/66  CLCN                 J 6/61  CLO                  J 3/61  CLO2                 J 9/65  CL2                  J12/65  CL2O
 J 6/73  CR                   J12/73  CRN                  J12/73  CRO                  J12/73  CRO2                 J12/73  CRO3
 J 6/77  CU                   J 3/66  CUCL                 J12/77  CUO                  J 9/66  CU2                  J 3/66  CU3CL3
 J 3/77  H                    J 3/64  HALO                 L12/69  HCN                  J12/70  HCO RAD              J 9/64  HCL
 J12/70  HNCO                 RUS 78  HNO                  RUS 78  HNO2                 RUS 78  HNO3                 J 3/79  HOCL
 J 9/78  HO2                  J 3/77  H2                   J12/65  H2N2                 J 3/79  H2O                  L 3/85  H2O2
 J 3/77  N                    J12/70  NCO                  RUS 78  NH                   RUS 78  NH2                  J 6/77  NH3
 RUS 78  NH2OH                RUS 78  NO                   RUS 78  NOCL                 RUS 78  NO2                  RUS 78  NO2CL
 J12/64  NO3                  J 3/77  N2                   RUS 78  N2H2                 RUS 78  NH2NO2               RUS 78  N2H4
 RUS 78  N2O                  RUS 78  N2O3                 RUS 78  N2O4                 RUS 78  N2O5                 RUS 78  N3
 RUS 78  N3H                  J 3/77  O                    J 6/77  OH                   J 3/77  O2                   J 6/61  O3
 J 6/79  AL(S)                J 6/79  AL(L)                J 9/79  ALCL3(S)             J 9/79  ALCL3(L)             J12/79  ALN(S)
 J12/79  AL2O3(A)             J12/79  AL2O3(L)             J12/70  BA(A)                J12/70  BA(B)                J12/70  BA(C)
 J12/70  BA(L)                J12/72  BACL2(A)             J12/72  BACL2(B)             J12/72  BACL2(L)             J 6/74  BAO(S)
 J 6/74  BAO(L)               J12/75  BAO2H2(S)            J12/75  BAO2H2(L)            J 3/78  C(GR)                P10/80  BENZENE(L)
 P10/80  TOLUENE(L)           P10/80  OCTANE(L)            L 8/86  JET-A(L)             J 6/73  CR(S)                J 6/73  CR(L)
 J12/73  CRN(S)               J12/73  CR2N(S)              J12/73  CR2O3(S)             J12/73  CR2O3(L)             J 6/77  CU(S)
 J 6/77  CU(L)                J12/77  CUO(S)                 6/66  CUO2H2(S)            J12/77  CU2O(S)              J12/77  CU2O(L)
 L 3/81  H2O(S)               J 3/79  H2O(L)               BAR73   NH4CL(A)             BAR73   NH4CL(B)
$RKTINP
EOL      = T.
FROZ     = T.
SUBAR    = 13*0.00000000000000000E+00,
SUPAR    =    7.2000000000000000    .   10.000000000000000    .
  15.300000000000000    .    20.000000000000000    . 9*0.00000000000000000E+00.
PCP      = 22*0.00000000000000000E+00,
TCEST    =    3800.000    .
NFZ      =               1
$END

OF =   0.000000
                          EFFECTIVE FUEL          EFFECTIVE OXIDANT           MIXTURE
ENTHALPY                     HPP(2)                    HPP(1)                   HSUB0
(KG-MOL)(DEG K)/KG      -0.26506627E+03           0.00000000E+00           -0.26506627E+03

KG-FORM.WT./KG              BOP(I,2)                  BOP(I,1)                  BO(I)
N                        0.63082801E-02            0.00000000E+00            0.63082801E-02
O                        0.26627772E-01            0.00000000E+00            0.26627772E-01
H                        0.44108626E-01            0.00000000E+00            0.44108626E-01
CL                       0.81801988E-02            0.00000000E+00            0.81801988E-02
C                        0.10731153E-01            0.00000000E+00            0.10731153E-01
AL                       0.36783710E-03            0.00000000E+00            0.36783710E-03
BA                       0.18866738E-04            0.00000000E+00            0.18866738E-04
CO                       0.18866738E-04            0.00000000E+00            0.18866738E-04
CU                       0.65909301E-04            0.00000000E+00            0.65909301E-04
CR                       0.65909301E-04            0.00000000E+00            0.65909301E-04

SINGULAR MATRIX, ITERATION  1  VARIABLE  8

SINGULAR MATRIX, ITERATION  2  VARIABLE  8
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SINGULAR MATRIX, ITERATION  3  VARIABLE  6

SINGULAR MATRIX, ITERATION  4  VARIABLE 10

WARNING--POINT  1  USES A REDUCED SET OF COMPONENTS AND NO SPECIES USING THE ELIMINATED COMPONENT ARE CALCULATED.
IF QUESTIONABLE, RERUN WITH INSERTED CONDENSED SPECIES CONTAINING COMPONENT CO

POINT ITN    T       N3H            O3             OH             NO2CL          NCO            NALO           BAO2H2
   CRO3              CU3CL3
  1   25 2647.56  -46.597         -55.490        -27.137        -69.871        -42.849        -45.687        -88.721
   -64.691           -94.458
ADD AL2O3(L)
  1    5 2679.09  -46.687         -55.233        -27.854        -68.787        -42.847        -49.375        -88.674
   -64.660           -94.749
ADD CR2O3(L)
  1    4 2694.85  -46.726         -55.874        -27.818        -68.678        -42.846        -49.247        -88.515
   -67.459           -94.895

SINGULAR MATRIX, ITERATION  1  VARIABLE 10

SINGULAR MATRIX, ITERATION  2  VARIABLE 16

SINGULAR MATRIX, ITERATION  3  VARIABLE 18

SINGULAR MATRIX, ITERATION  4  VARIABLE 10

WARNING--POINT  2  USES A REDUCED SET OF COMPONENTS AND NO SPECIES USING THE ELIMINATED COMPONENT ARE CALCULATED.
IF QUESTIONABLE, RERUN WITH INSERTED CONDENSED SPECIES CONTAINING COMPONENT CO

POINT ITN    T       N2             CO2            H2O            HCL            CO             AL2O3(L)       BACL2
   CR2O3(L)          CUCL
  2   10 2436.97  -25.596         -50.300        -36.986        -28.573        -30.906        -105.521       -75.347
   -83.195           -31.353
PHASE CHANGE, REPLACE CR2O3(L)         WITH CR2O3(S)
  2    2 2439.07  -25.599         -50.289        -36.988        -28.572        -30.964        -105.466       -75.331
   -83.563           -31.368
PC/PT= 1.780411    T =  2439.07

SINGULAR MATRIX, ITERATION  1  VARIABLE 10

SINGULAR MATRIX, ITERATION  2  VARIABLE 10

SINGULAR MATRIX, ITERATION  3  VARIABLE 10

SINGULAR MATRIX, ITERATION  4  VARIABLE 10

WARNING--POINT  2  USES A REDUCED SET OF COMPONENTS AND NO SPECIES USING THE ELIMINATED COMPONENT ARE CALCULATED.
IF QUESTIONABLE, RERUN WITH INSERTED CONDENSED SPECIES CONTAINING COMPONENT CO

POINT ITN    T       N2             CO2            H2O            HCL            CO             AL2O3(L)       BACL2
   CR2O3(S)          CUCL
  2    9 2437.05  -25.601         -50.305        -36.911        -28.578        -30.911        -105.519       -75.351
   -83.598           -31.358
PC/PT= 1.788686    T =  2437.05

SINGULAR MATRIX, ITERATION  1  VARIABLE 10

SINGULAR MATRIX, ITERATION  2  VARIABLE 10

SINGULAR MATRIX, ITERATION  3  VARIABLE 10

SINGULAR MATRIX, ITERATION  4  VARIABLE 10

WARNING--POINT  2  USES A REDUCED SET OF COMPONENTS AND NO SPECIES USING THE ELIMINATED COMPONENT ARE CALCULATED.
IF QUESTIONABLE, RERUN WITH INSERTED CONDENSED SPECIES CONTAINING COMPONENT CO
  2    9 2437.04  -25 601         -50.305        -36.911        -28.578        -30.911        -105.519       -75 351
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   -83.599         -31.358
PC/PI= 1.788749   T =  2437.84

SINGULAR MATRIX, ITERATION  1  VARIABLE 10

SINGULAR MATRIX, ITERATION  2  VARIABLE 10

SINGULAR MATRIX, ITERATION  3  VARIABLE 10

SINGULAR MATRIX, ITERATION  4  VARIABLE 10

WARNING--POINT  3  USES A REDUCED SET OF COMPONENTS AND NO SPECIES USING THE ELIMINATED COMPONENT ARE CALCULATED.
IF QUESTIONABLE, RERUN WITH INSERTED CONDENSED SPECIES CONTAINING COMPONENT CO
  3   13 1284.82  -26.929          -67.251         -48.526         -34.831         -37.390         -168.494         -97.138
  -125.767         -31.818
PHASE CHANGE, REPLACE AL2O3(L)          WITH AL2O3(A)
  3    2 1286.64  -26.933          -67.207         -48.493         -34.823         -37.378         -171.472         -97.080
  -125.633         -31.813
ADD BACL2(L)
  3    4 1289.47  -26.939          -67.139         -48.456         -34.818         -37.360         -171.158        -101 842
  -125.429         -31.805

SINGULAR MATRIX, ITERATION  1  VARIABLE 10

SINGULAR MATRIX, ITERATION  2  VARIABLE 10

SINGULAR MATRIX, ITERATION  3  VARIABLE 10

SINGULAR MATRIX, ITERATION  4  VARIABLE 10

WARNING--POINT  3  USES A REDUCED SET OF COMPONENTS AND NO SPECIES USING THE ELIMINATED COMPONENT ARE CALCULATED.
IF QUESTIONABLE, RERUN WITH INSERTED CONDENSED SPECIES CONTAINING COMPONENT CO

POINT ITN   T       H2              CO2             H2S             HCL             CO              AL2O3(A)        BACL2(L)
   CA2O3(S)         CU3CL3
  3   11 1281 21  -26.953          -67.371         -48.613         -34.888         -37.446         -172.890        -102.283
  -126.035         -93.118

SINGULAR MATRIX, ITERATION  1  VARIABLE 10

SINGULAR MATRIX, ITERATION  2  VARIABLE 10

SINGULAR MATRIX, ITERATION  3  VARIABLE 10

SINGULAR MATRIX, ITERATION  4  VARIABLE 10

WARNING--POINT  3  USES A REDUCED SET OF COMPONENTS AND NO SPECIES USING THE ELIMINATED COMPONENT ARE CALCULATED.
IF QUESTIONABLE, RERUN WITH INSERTED CONDENSED SPECIES CONTAINING COMPONENT CO
  3   11 1281.26  -26.953          -67.370         -48.613         -34.880         -37.445         -172.885        -102.281
  -126.332         -93.118

SINGULAR MATRIX, ITERATION  1  VARIABLE 10

SINGULAR MATRIX, ITERATION  2  VARIABLE 10

SINGULAR MATRIX, ITERATION  3  VARIABLE 10

SINGULAR MATRIX, ITERATION  4  VARIABLE 10

WARNING--POINT  4  USES A REDUCED SET OF COMPONENTS AND NO SPECIES USING THE ELIMINATED COMPONENT ARE CALCULATED.
IF QUESTIONABLE, RERUN WITH INSERTED CONDENSED SPECIES CONTAINING COMPONENT CO
  4   11 1173.50  -27 159          -78.729         -50.891         -35.887         -38.684         -185.610        -108.712
  -134.835         -94.710
PHASE CHANGE, REPLACE BACL2(L)          WITH BACL2(B)
  4    2 1173.68  -27.159          -78.724         -50.888         -35.886         -38.682         -185.[illegible]6        -108.785
  -134.819         -94.707
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ADD BACL2(A)
  4    3 1197.99  -27.217          -70.018         -58.444         -34.958         -38.490         -182.312        -107.189
  -132.684         -94.420
REMOVE BACL2(B)
  4    2 1173.85  -27.160          -70.719         -58.885         -35.885         -38.681         -185.562        -108.807
  -134.804         -94.705
ADD CU(S)
  4    3 1173.89  -27.160          -70.718         -58.884         -35.884         -38.681         -185.557        -108.805
  -134.800         -94.802

SINGULAR MATRIX, ITERATION  1  VARIABLE 10

SINGULAR MATRIX, ITERATION  2  VARIABLE 10

SINGULAR MATRIX, ITERATION  3  VARIABLE 10

SINGULAR MATRIX, ITERATION  4  VARIABLE 10

WARNING--POINT  4  USES A REDUCED SET OF COMPONENTS AND NO SPECIES USING THE ELIMINATED COMPONENT ARE CALCULATED.
IF QUESTIONABLE, RERUN WITH INSERTED CONDENSED SPECIES CONTAINING COMPONENT CO

POINT ITN   T      N2              CO2             H2O             HCL             CO              AL2O3(A)        BACL2(A)
   CR2O3(S)        CU3CL3
  4   11 1175.36  -27.157          -70.668         -58.850         -35.869         -38.662         -185.355        -108.704
  -134.668         -94.770

SINGULAR MATRIX, ITERATION  1  VARIABLE 10

SINGULAR MATRIX, ITERATION  2  VARIABLE 10

SINGULAR MATRIX, ITERATION  3  VARIABLE 10

SINGULAR MATRIX, ITERATION  4  VARIABLE 10

WARNING--POINT  5  USES A REDUCED SET OF COMPONENTS AND NO SPECIES USING THE ELIMINATED COMPONENT ARE CALCULATED.
IF QUESTIONABLE, RERUN WITH INSERTED CONDENSED SPECIES CONTAINING COMPONENT CO
  5   11 1059.09  -27.419          -75.074         -53.832         -36.371         -40.288         -203.141        -117.586
  -146.302         -97.630

SINGULAR MATRIX, ITERATION  1  VARIABLE 10

SINGULAR MATRIX, ITERATION  2  VARIABLE 10

SINGULAR MATRIX, ITERATION  3  VARIABLE 10

SINGULAR MATRIX, ITERATION  4  VARIABLE 10

WARNING--POINT  5  USES A REDUCED SET OF COMPONENTS AND NO SPECIES USING THE ELIMINATED COMPONENT ARE CALCULATED.
IF QUESTIONABLE, RERUN WITH INSERTED CONDENSED SPECIES CONTAINING COMPONENT CO

POINT ITN   T      N2              CO2             H2O             HCL             CO              AL2O3(A)        BACL2(A)
   CR2O3(S)        CU(S)
  5   10 1059.29  -27.418          -75.066         -53.826         -36.368         -40.284         -203.107        -117.569
  -146.286          -5.695

SINGULAR MATRIX, ITERATION  1  VARIABLE 10

SINGULAR MATRIX, ITERATION  2  VARIABLE 10

SINGULAR MATRIX, ITERATION  3  VARIABLE 10

SINGULAR MATRIX, ITERATION  4  VARIABLE 10

WARNING--POINT  6  USES A REDUCED SET OF COMPONENTS AND NO SPECIES USING THE ELIMINATED COMPONENT ARE CALCULATED.
IF QUESTIONABLE, RERUN WITH INSERTED CONDENSED SPECIES CONTAINING COMPONENT CO
  6   11  985.87  -27.615          -78.405         -56.080         -37.347         -41.521         -216.593        -124.327
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 -155.137         -5.532

SINGULAR MATRIX, ITERATION  1  VARIABLE 18

SINGULAR MATRIX, ITERATION  2  VARIABLE 18

SINGULAR MATRIX, ITERATION  3  VARIABLE 18

SINGULAR MATRIX, ITERATION  4  VARIABLE 18

WARNING--POINT  6  USES A REDUCED SET OF COMPONENTS AND NO SPECIES USING THE ELIMINATED COMPONENT ARE CALCULATED.
IF QUESTIONABLE, RERUN WITH INSERTED CONDENSED SPECIES CONTAINING COMPONENT CO

POINT ITN   T      H2              CO2             N2              HCL             CO              AL2O3(A)        BACL2(A)
  CR2O3(S)         CU(S)
 6   11  986.46  -27.613          -78.376         -19.195         -37.339         -41.510         -216.477        -124.268
 -155.861          -5.333
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THEORETICAL ROCKET PERFORMANCE ASSUMING EQUILIBRIUM COMPOSITION DURING EXPANSION

PC = 2500.0 PSIA
CASE NO. 208

	CHEMICAL FORMULA				WT FRACTION (SEE NOTE)	ENERGY CAL/MOL	STATE	TEMP DEG K
FUEL	N 1.00000	O 4.00000	H 4.00000	CL 1.00000	0.741153	-70580.000	S	298.15
FUEL	C 2.00000	CL 1.00000	H 3.00000		0.116992	8400.000	S	298.15
FUEL	C 22.00000	O 4.00000	H 42.00000		0.116992	-300000.000	S	298.15
FUEL	C 1.00000				0.008501	0.000		0.00
FUEL	AL 1.00000				0.009925	0.000		0.00
FUEL	BA 1.00000	CO 1.00000			0.004712	0.000		0.00
FUEL	CU 2.00000	CR 2.00000	O 4.00000		0.009724	0.000		0.00

O/F= 0.0000 PERCENT FUEL= 100.0000 EQUIVALENCE RATIO= 1.4412 PHI= 0.0000

	CHAMBER	THROAT	EXIT	EXIT	EXIT	EXIT
PC/P	1.0000	1.7807	55.782	87.422	158.76	220.58
P, ATM	170.11	95.102	3.0496	1.9459	1.1204	0.77121
T, DEG K	2694.9	2437.0	1281.3	1175.4	1059.3	986.5
RHO, G/CC	1.9161-2	1.1060-2	7.2512-4	5.0439-4	3.2454-4	2.3024-4
H, CAL/G	-526.74	-645.66	-1140.46	-1184.38	-1232.65	-1263.57
U, CAL/G	-741.74	-839.85	-1242.31	-1277.73	-1316.85	-1341.97
G, CAL/G	-6668._8	-6199.73	-4066.48	-3862.98	-3646.79	-3511.74
S, CAL/(G)(K)	2.2790	2.2790	2.2790	2.2790	2.2790	2.2790
M, MOL WT	24.987	24.939	24.999	25.000	25.000	25.006
(DLV/DLP)T	-1.00126	-1.00052	-1.00007	-1.00019	-1.00032	-1.00006
(DLV/DLT)P	1.0255	1.0111	1.0014	1.0087	1.0029	1.0113
CP, CAL/(G)(K)	0.4717	0.4425	0.4053	0.4071	0.4142	0.4285
GAMMA (S)	1.2145	1.2240	1.2447	1.2425	1.2307	1.2328
SON VEL,M/SEC	1045.2	997.6	728.3	696.9	668.6	655.9
MACH NUMBER	0.000	1.000	3.112	3.366	3.679	3.985

PERFORMANCE PARAMETERS

AE/AT	1.0000	7.2000	10.000	15.000	20.000
CSTAR, FT/SEC	4780	4780	4780	4780	4780
CF	0.685	1.556	1.610	1.662	1.704
IVAC,LB-SEC/LB	184.0	250.3	256.2	262.6	266.7
ISP, LB-SEC/LB	101.7	231.1	239.2	247.8	253.2

MOLE FRACTIONS

ALCL	1.454 -5	3.060 -6	1.607-14	3.486-16	2.868-18	4.334-20
ALCL2	5.648 -5	1.641 -5	4.804-12	2.494-13	4.862-15	2.523-16
ALCL3	1.529 -4	8.335 -5	2.942 -8	6.694 -9	9.624-10	2.268-10
ALOCL	2.971 -5	7.013 -6	1.288-13	3.622-15	3.865-17	8.457-19
ALOH	1.525 -6	2.797 -7	4.400-16	7.779-18	3.419-20	5.730-22
ALO2H	1.217 -5	2.367 -6	6.491-15	1.311-16	6.020-19	1.309-20
BACL2	4.6629-4	4.6757-4	3.1754-6	3.4871-7	1.3434-8	1.1163-9
BAO2H2	1.001 -6	3.755 -7	3.472-13	7.245-15	3.891-17	4.991-19
FORMALDEHYDE	2.6599-6	1.5480-6	8.2519-8	5.7407-8	3.6581-8	2.6372-8
FORMIC ACID	3.9155-6	2.1387-6	7.6453-8	5.1145-8	3.1456-8	2.2358-8
CH4	8.0207-8	7.4226-8	3.6586-6	1.1657-5	5.0285-5	1.9961-4
CO	1.9815-1	1.9472-1	1.4681-1	1.3536-1	1.1945-1	1.0732-1
COCL	8.048 -6	2.934 -6	5.380-10	1.122-10	1.458-11	3.182-12
CO2	6.7727-2	7.1474-2	1.2988-1	1.3129-1	1.4697-1	1.5895-1
CL	1.576 -3	7.275 -4	1.817 -7	3.442 -8	3.735 -9	7.841-10
CLO	5.204 -7	7.967 -8	5.227-16	1.321-17	9.932-20	2.551-21
CL2	1.569 -5	6.028 -6	9.322-10	1.771-10	1.982-11	3.876-12
CP	1.713 -5	2.662 -6	1.926-15	2.683-17	8.583-20	1.118-21

CRO	4.624 -5	5.890 -6	4.896-16	4.454-18	8.119-21	6.966-23
CRO2	3.226 -5	4.153 -6	3.651-16	3.370-18	6.308-21	5.539-23
CU	9.374 -5	6.183 -5	2.849 -9	3.132 -9	1.308-10	1.165-11
CUCL	1.5388-3	1.5722-3	1.8594-4	3.3887-5	5.6463-6	1.4772-6
CU3CL3	8.5336-8	2.8719-7	5.1868-4	4.8878-4	2.6622-4	1.7891-4
H	1.567 -3	7.707 -4	2.814 -7	3.921 -8	4.385 -9	8.430-10
HCN	2.6716-6	1.5334-6	7.5671-8	5.2147-8	3.2851-8	2.3485-8
HCO RAD	5.766 -6	2.882 -6	3.761-10	7.929-11	1.813-11	2.173-12
HCL	1.9798-1	1.9938-1	2.0872-1	2.0884-1	2.0139-1	2.0137-1
HNCO	9.1218-7	4.7244-7	8.2632-9	4.6738-9	2.2764-9	1.3486-9
HOCL	3.669 -6	9.894 -7	4.315-12	4.124-13	1.845-14	2.815-15
H2	1.3676-1	1.4029-1	1.8869-1	2.0881-1	2.1515-1	2.2655-1
H2O	3.0941-1	3.0656-1	2.5985-1	2.4758-1	2.3169-1	2.1583-1
NH2	1.892 -6	3.189 -7	2.833-11	3.682-12	3.699-13	6.008-14
NH3	2.1912-5	1.6321-5	9.6149-6	1.0736-5	1.2947-5	1.5182-5
NO	5.373 -5	1.370 -5	1.159-11	7.341-13	1.852-14	1.174-15
N2	7.8113-2	7.8227-2	7.8383-2	7.8375-2	7.8319-2	7.8324-2
O	6.644 -6	1.839 -6	3.426-15	6.984-17	3.735-19	7.481-21
OH	9.240 -4	3.898 -4	3.422 -9	3.512-10	1.673-11	1.780-12
O2	6.118 -6	9.418 -7	2.326-15	4.364-17	2.161-19	4.817-21
AL2O3(A)	0.0000 0	0.0000 0	4.5708-3	4.5784-3	4.5672-3	4.5669-3
AL2O3(L)	4.4235-3	4.5861-3	0.0000 0	0.0000 0	0.0000 0	0.0000 0
BACL2(A)	0.0000 0	0.0000 0	0.0000 0	4.6849-4	4.6858-4	4.6849-4
BACL2(L)	0.0000 0	0.0000 0	4.6571-4	0.0000 0	0.0000 0	0.0000 0
CR2O3(S)	0.0000 0	8.1113-4	8.1900-4	8.1892-4	8.1835-4	8.1831-4
CR2O3(L)	7.6869-4	0.0000 0	0.0000 0	0.0000 0	0.0000 0	0.0000 0
CU(S)	0.0000 0	0.0000 0	0.0000 0	1.3842-4	8.3239-4	1.1224-3

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.50000E-06 FOR ALL ASSIGNED CONDITIONS

AL	ALC	ALH	ALN	ALO	ALO2	AL2
AL2CL6	AL2O	AL2O2	BA	BACL	BAOH	C
CCL	CCL2	CCL3	CCL4	CH	CHCL	CHCL3
CH2	CH2CL2	CH3	CH3CL	HYDROXYMETHYLENE	METHYLOXIDE	METHANOL
CN	NCN RAD	CNN RAD	COCL2	C2	C2CL2	C2CL4
C2CL6	C2H RAD	C2HCL	ACETYLENE	KETENE	C2H3 RAD	METHYL CYANIDE
CH3CO RAD	CH2CHO RAD	ETHYLENE	ACETALDEHYDE	ACETIC ACID	(FORMIC ACID)2	ETHYL RAD
ETHYL OXIDE RAD	ETHANE	AZOMETHANE	DIMETHYL ETHER	ETHANOL	CNC RAD	CYANOGEN
CCO RAD	C3	C3H3 RAD	CYCLOPROPENE	PROPYNE	ALLENE	C3H5 RAD
CYCLOPROPANE	PROPYLENE	PROPYLENE OXIDE	I-PROPYL RAD	N-PROPYL RAD	PROPANE	1-PROPANOL
CARBON SUBOXIDE	C4	BUTADIYNE	CYCLOBUTADIENE	BUTAN-1EN-3YN	1,3-BUTADIENE	2-BUTYNE
2-BUTENE TRANS	2-BUTENE CIS	ISOBUTENE	1-BUTENE	(ACETIC ACID)2	T-BUTYL RAD	S-BUTYL RAD
N-BUTYL RAD	N-BUTANE	ISOBUTANE	CARBON SUBNITRIDE	C5	CYCLOPENTADIENE	CYCLOPENTANE
1-PENTENE	T-PENTYL RAD	N-PENTYL RAD	PENTANE	ISOPENTANE	CH3C(CH3)2CH3	HEXATRIYNE
PHENYL RAD	PHENOXY RAD	BENZENE	PHENOL	CYCLOHEXENE	N-HEXYL RAD	TOLUENE
CRESOL	1-HEPTENE	N-HEPTYL RAD	N-HEPTANE	1-OCTENE	N-OCTYL RAD	OCTANE
ISO-OCTANE	N-NONYL RAD	NAPTHLENE	AZULENE	N-DECYL RAD	O-BIPHENYL RAD	BIPHENYL
JET-A(G)	CLCN	CLO2	CL2O	CRN	CRO3	CUO
CU2	HALO	HNO	HNO2	HNO3	HO2	N2H2
H2O2	N	NCO	NH	NH2OH	NOCL	NO2
NO2CL	NO3	N2H2	NH2NO2	N2H4	N2O	N2O3
N2O4	N2O5	N3	N3H	O3	AL(S)	AL(L)
ALCL3(S)	ALCL3(L)	ALN(S)	BA(A)	BA(B)	BA(C)	BA(L)
BACL2(B)	BAO(S)	BAO(L)	BAO2H2(S)	BAO2H2(L)	C(GR)	BENZENE(L)
TOLUENE(L)	OCTANE(L)	JET-A(L)	CR(S)	CR(L)	CRN(S)	CR2N(S)
CU(L)	CUO(S)	CUO2H2(S)	CU2O(S)	CU2O(L)	H2O(S)	H2O(L)
NH4CL(A)	NH4CL(B)					

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

THEORETICAL ROCKET PERFORMANCE ASSUMING FROZEN COMPOSITION DURING EXPANSION

PC = 2500.0 PSIA
CASE NO. 200

	CHEMICAL FORMULA				WT FRACTION (SEE NOTE)	ENERGY CAL/MOL	STATE	TEMP DEG K
FUEL	N 1.00000	O 4.00000	H 4.00000	CL 1.00000	0.741153	-70580.000	S	298.15
FUEL	C 2.00000	CL 1.00000	H 3.00000		0.116992	8480.000	S	298.15
FUEL	C 22.00000	O 4.00000	H 42.00000		0.116992	-389000.000	S	298.15
FUEL	C 1.00000				0.006561	0.000		0.00
FUEL	AL 1.00000				0.009925	0.000		0.00
FUEL	BA 1.00000	CO 1.00000			0.004712	0.000		0.00
FUEL	CU 2.00000	CR 2.00000	O 4.00000		0.009724	0.000		0.00

O/F= 0.0000 PERCENT FUEL= 100.0000 EQUIVALENCE RATIO= 1.4412 PHI= 0.0000

	CHAMBER	THROAT
PC/P	1.0000	
P, ATM	170.11	
T, DEG K	2694.9	
RHO, G/CC	1.9161-2	
H, CAL/G	-526.74	
U, CAL/G	-741.74	
G, CAL/G	-6668.38	
S, CAL/(G)(K)	2.2796	
M, MOL WT	24.987	
CP, CAL/(G)(K)	0.4227	
GAMMA (S)	1.2326	
SON VEL,M/SEC	1053.8	
MACH NUMBER	0.000	

PERFORMANCE PARAMETERS

AE/AT
CSTAR, FT/SEC
CF
IVAC,LB-SEC/LB
ISP, LB-SEC/LB

MOLE FRACTIONS

ALCL	0.00001	ALCL2	0.00006	ALCL3	0.00015	ALOCL	0.00003
ALOH	0.00000	ALO2H	0.00001	BACL2	0.00047	BAO2H2	0.00000
FORMALDEHYDE	0.00000	FORMIC ACID	0.00000	CO	0.19815	COCL	0.00001
CO2	0.06773	CL	0.00158	CLO	0.00000	CL2	0.00002
CN	0.00002	CRO	0.00005	CRO2	0.00003	CU	0.00009
CUCL	0.00154	H	0.00157	HCN	0.00000	HCO RAD	0.00001
HCL	0.19798	HNCO	0.00002	HOCL	0.00030	H2	0.13676
H2O	0.30941	NH2	0.00000	NH3	0.00002	NO	0.00005
N2	0.07811	O	0.00001	OH	0.00072	O2	0.00001
AL2O3(L)	0.06442	CR2O3(L)	0.00077				

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.50000E-05 FOR ALL ASSIGNED CONDITIONS

AL	ALC	ALN	ALO	ALO2	AL2	
AL2CL6	AL2O	AL2O2	BA	BACL	BAOH	C
CCL	CCL2	CCL3	CCL4	CH	CHCL	CHCL3
CH2	CH2CL2	CH3	CH3CL	HYDROXYMETHYLENE	METHYLOXIDE	CH4
METHANOL	CN	NCN RAD	CNN RAD	COCL2	C2	C2CL2
C2CL4	C2CL6	C2N RAD	C2HCL	ACETYLENE	KETENE	C2H3 RAD
METHYL CYANIDE	CH3CO RAD	CH2CHO RAD	ETHYLENE	ACETALDEHYDE	ACETIC ACID	(FORMIC ACID)2
ETHYL RAD	ETHYL OXIDE RAD	ETHANE	AZOMETHANE	DIMETHYL ETHER	ETHANOL	CNC RAD

CYANOGEN	CCO RAD	C3	C3H3 RAD	CYCLOPROPENE	PROPYNE	ALLENE
C3H5 RAD	CYCLOPROPANE	PROPYLENE	PROPYLENE OXIDE	1-PROPYL RAD	N-PROPYL RAD	PROPANE
1-PROPANOL	CARBON SUBOXIDE	C4	BUTADIYNE	CYCLOBUTADIENE	BUTAN-1EN-3YN	1.3-BUTADIENE
2-BUTYNE	2-BUTENE TRANS	2-BUTENE CIS	ISOBUTENE	1-BUTENE	(ACETIC ACID)2	T-BUTYL RAD
S-BUTYL RAD	N-BUTYL RAD	N-BUTANE	ISOBUTANE	CARBON SUBNITRID	C5	CYCLOPENTADIENE
CYCLOPENTANE	1-PENTENE	T-PENTYL RAD	N-PENTYL RAD	PENTANE	ISOPENTANE	CH3C(CH3)2CH3
HEXATRIYNE	PHENYL RAD	PHENOXY RAD	BENZENE	PHENOL	CYCLOHEXENE	N-HEXYL RAD
TOLUENE	CRESOL	1-HEPTENE	N-HEPTYL RAD	N-HEPTANE	1-OCTENE	N-OCTYL RAD
OCTANE	ISO-OCTANE	N-NONYL RAD	NAPTHLENE	AZULENE	N-DECYL RAD	O-BIPHENYL RAD
BIPHENYL	JET-A(G)	CLCN	CLO2	CL2O	CRN	CRO3
CUO	CU2	CH3CL3	HALO	HNO	HNO2	HNO3
HO2	H2N2	H2O2	N	NCO	NH	NH2OH
HOCL	NO2	NO2CL	NO3	N2H2	NH2NO2	N2H4
H2O	N2O3	N2O4	N2O5	N3	N3H	O3
AL(S)	AL(L)	ALCL3(S)	ALCL3(L)	ALN(S)	AL2O3(A)	NA(A)
BA(B)	BA(C)	BA(L)	BACL2(A)	BACL2(B)	BACL2(L)	BAO(S)
BAO(L)	BAO2H2(S)	BAO2H2(L)	C(GR)	BENZENE(L)	TOLUENE(L)	OCTANE(L)
JET-A(L)	CR(S)	CR(L)	CRN(S)	CR2N(S)	CR2O3(S)	CU(S)
CU(L)	CUO(S)	CUO2H2(S)	CU2O(S)	CU2O(L)	H2O(S)	H2O(L)
NH4CL(A)	NH4CL(B)					

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

CALCULATIONS WERE STOPPED BECAUSE NEXT POINT IS MORE THAN 50 DEG BELOW TEMP RANGE OF A CONDENSED SPECIES

Table C-4

NASA - Lewis CET - 86

Output

Composition Q

Tue Dec 3 18:16:49 CDT 1991

CWN

COMPQ.LAS

REACTANTS

C	3.0000	O	9.0000	H	5.0000	N	3.0000	0.0000	11.360000	-85300.00	S	298.150
C	4.0000	O	9.0000	H	7.0000	N	3.0000	0.0000	11.360000	-93070.00	S	298.150
C	4.0000	O	8.0000	H	8.0000	N	8.0000	0.0000	66.600000	17930.00	S	298.150
C	10.0000	O	5.0000	H	16.0000		0.0000	0.0000	4.630000	-282980.00	S	298.150
C	2.0000	O	1.0000	H	3.0000	N	1.0000	0.0000	1.600000	-23556.00	S	298.150
C	7.0000	O	2.0000	H	8.0000	N	2.6000	0.0000	0.750000	-7460.00	S	298.150
C	12.0000	O	2.0000	H	11.0000	N	2.0000	0.0000	0.400000	-15400.00	S	298.150
C	6.0000	O	7.0000	H	8.0000		0.0000	0.0000	0.340000	-655130.00	S	298.150
C	12.0000	O	20.0000	H	15.0000	N	5.0000	0.0000	0.340000	-160200.00	S	298.150
ZN	1.0000	C	1.0000		0.0000		0.0000	0.0000	1.000000	-40500.00	S	298.150
PB	3.0000	C	12.0000	H	16.0000	O	17.0000	0.0000	1.500000	0.00	S	298.150
C	1.0000		0.0000		0.0000		0.0000	0.0000	0.400000	0.00	S	298.150
BI	1.0000	C	10.0000	H	15.0000		0.0000	0.0000	0.040000	0.00	S	298.150

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NAMELISTS
$INPT2
KASE    =         300,
T       = 26*0.0000000E-00,
P       =    1400.000    , 25*0.0000000E+00,
PSIA    = T,
NMMG    = F,
NSON    = F,
V       = 26*0.0000000E+00,
RHO     =    1400.000    , 25*0.0000000E+00,
ERATIO  = F,
OF      = F,
FPCT    = F,
FA      = F,
MIX     = 26*-1.000000     ,
TP      = F,
HP      = F,
SP      = F,
TV      = F,
UV      = F,
SV      = F,
RKT     = T,
SHOCK   = F,
DETN    = F,
TRACE   =  5.0000000000000000E-07,
SO      =  0.0000000000000000E+00,
SO      =  0.0000000E+00,
IONS    = F,
IDEBUG  =           0,
PHI     = F,
SIUNIT  = F,
INMG    = F,
TRNSPT  = F,
TRPACC  =  0.999900000000000     ,
DIF     = F,
NODATA  = F,
U       =  1.0000000000000000E+30,
H       =  1.0000000000000000E+30
$END
```

NO INPT2 VALUE GIVEN FOR OF, ERAT, FA, OR FPCT

SPECIES BEING CONSIDERED IN THIS SYSTEM

L 7/75	BI	J 3/78	C	J12/67	CH	J12/72	CH2	J 3/61	FORMALDEHYDE
L 4/85	FORMIC ACID	J 6/69	CH3	L 9/85	HYDROXYMETHYLENE	L 9/85	METHYLOXIDE	L 5/84	CH4
L 9/85	METHANOL	J 6/69	CN	J12/70	HCN RAD	J 6/66	CHN RAD	J 9/65	CO
J 9/65	CO2	J12/69	C2	J 3/67	C2H CAD	J 3/61	ACETYLENE	BUR 84	KETENE
BUR 84	C2H3 RAD	BUR 84	METHYL CYANIDE	BUR 84	CH3CO RAD	BUR 84	CH2CHO RAD	L 4/85	ETHYLENE
BUR 84	ACETALDEHYDE	L 4/85	ACETIC ACID	L 4/85	(FORMIC ACID)2	P10/85	ETHYL RAD	BUR 84	ETHYL OXIDE RAD

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 L 5/84   ETHANE             BUR 84   AZOMETHANE         BUR 84   DIMETHYL ETHER     BUR 84   ETHANOL            J 3/67   CNC RAD
 J 3/61   CYANOGEN           J 9/66   CCN RAD            J12/69   C3                 D06/61   C3H3 RAD           BUR 84   CYCLOPROPENE
 BUR 84   PROPYNE            BUR 84   ALLENE             BUR 8C   C3H5 RAD           BUR 84   CYCLOPROPANE       L 4/85   PROPYLENE
 L 9/85   PROPYLENE OXIDE    L 9/85   I-PROPYL RAD       L 9/85   N-PROPYL RAD       L 4/85   PROPANE            L 1/84   2-PROPANOL
 J 6/68   CARBON SUBOXIDE    J12/69   C4                 BUR 84   BUTADIYNE          P10/85   CYCLOBUTADIENE     BUR 84   BUTAN-1EN-3YN
 F 4/84   1,3-BUTADIENE      BUR 84   2-BUTYNE           BUR 84   2-BUTENE TRANS     BUR 84   2-BUTENE CIS       BUR 84   ISOBUTENE
 BUR 84   1-BUTENE           L 4/85   (ACETIC ACID)2     L 9/85   T-BUTYL RAD        L 9/85   S-BUTYL RAD        P10/83   N-BUTYL RAD
 L 4/85   N-BUTANE           L 4/85   ISOBUTANE          J 3/61   CARBON SUBNITRID   J12/69   C5                 P10/85   CYCLOPENTADIENE
 P12/52   CYCLOPENTANE       P17/52   1-PENTENE          L 5/87   T-PENTYL RAD       P10/83   N-PENTYL RAD       P10/85   PLATANE
 P10/85   ISOPENTANE         P10/85   CH3C(CH3)2CH3      BUR 84   HEXATRIYNE         L12/84   PHENYL RAD         L12/84   PHENOXY RAD
 L12/84   BENZENE            L12/84   PHENOL             BUR 84   CYCLOHEXENE        P10/83   N-HEXYL RAD        P10/84   TOLUENE
 L 6/87   CRESOL             P12/52   1-HEPTENE          P10/83   N-HEPTYL RAD       P 4/81   N-HEPTANE          P12/52   1-OCTENE
 P10/83   N-OCTYL RAD        P 4/85   OCTANE             P 4/85   ISO-OCTANE         P10/83   N-NONYL RAD        BUR 84   NAPTHLENE
 BUR 84   AZULENE            P10/83   N-DECYL RAD        L12/84   O-BIPHENYL RAD     L12/84   BIPHENYL           L 6/88   JET-A(G)
 J 3/77   H                  L12/69   HCN                J12/70   HCO RAD            J12/70   HNCO               RUS 78   HNO
 RUS 78   HNO2               RUS 78   HNO3               J 9/78   HO2                J 3/77   H2                 J12/65   N2H2
 J 3/79   H2O                L 3/85   H2O2               J 3/77   N                  J12/70   NCO                RUS 78   NH
 RUS 78   NH2                J 6/77   NH3                RUS 78   NH2OH              RUS 78   NO                 RUS 78   NO2
 J12/64   NO3                J 3/77   N2                 RUS 78   N2H2               RUS 78   NH2NO2             RUS 78   N2H4
 RUS 78   N2O                RUS 78   N2O3               RUS 78   N2O4               RUS 78   N2O5               RUS 78   N3
 RUS 78   N3H                J 3/77   O                  J 6/77   OH                 J 3/77   O2                 J 6/61   O3
 J 3/62   PB                 J12/71   PBO                J 9/63   PB2                J 6/79   ZR                 J 6/67   ZRN
 J12/65   ZRO                J12/65   ZRO2               BAR 73   BI(S)              BAR 73   BI(L)              J 3/78   C(GR)
 P10/80   BENZENE(L)         P10/80   TOLUENE(L)         P10/80   OCTANE(L)          L 8/86   JET-A(L)           L 3/81   H2O(S)
 J 3/79   H2O(L)             J 3/62   PB(S)              J 3/62   PB(L)              J12/71   PBO(RD)            J12/71   PBO(YW)
 J12/71   PBO(L)             J12/71   PBO2(S)            J12/71   PB3O4(S)           J 6/79   ZR(A)              J 6/79   ZR(B)
 J 6/79   ZR(L)              J 6/61   ZRN(S)             J 6/61   ZRN(L)             J12/65   ZRO2(A)            J12/65   ZRO2(B)
 J12/65   ZRO2(L)
$PRTINP
EQL      = T,
FROZ     = T,
SUBAR    = 13*0.000000000000000E+00,
SUPAR    =    2.250000000000000    ,    3.130000000000000    ,
  4.250000000000000    ,    5.000000000000000    ,    6.250000000000000    ,
 8*0.000000000000000E+00,
PCP      = 22*0.000000000000000E+00,
TCEST    =    3800.000    ,
NFZ      =              1
$END

OF =    0.030000
                             EFFECTIVE FUEL         EFFECTIVE OXIDANT        MIXTURE
ENTHALPY                         HPP(2)                  HPP(1)                HSUB0
(KG-MOL)(DEG K)/KG          -0.67747022E+02         0.00000000E+00        -0.67747022E+02

KG-FORM WT./KG                  BOP(I,2)                BOP(I,1)                BO(I)
C                            0.16487766E-01         0.00000000E+00         0.16487766E-01
O                            0.28607715E-01         0.00000000E+00         0.28607715E-01
H                            0.29159593E-01         0.00000000E+00         0.29159593E-01
N                            0.21203800E-01         0.00000000E+00         0.21203800E-01
ZR                           0.96870128E-04         0.00000000E+00         0.96870128E-04
PB                           0.42700648E-04         0.00000000E+00         0.42700648E-04
BI                           0.90847787E-06         0.00000000E+00         0.90847787E-06

POINT ITN    T        CO          H2O          H2           N2          ZRO2         PB           BI

  1   20 2920.18  -30.116      -36.143      -18.137      -25.033      -55.063      -18.915      -23.540

ADD ZRO2(B)
  1    5 2955.30  -30.104      -36.083      -18.180      -25.076      -62.741      -19.044      -23.667

ADD ZRO2(L)
  1    1 2950.44  -30.105      -36.092      -18.174      -25.069      -62.801      -19.026      -23.649

REMOVE ZRO2(B)
  1    2 2951.31  -30.105      -36.090      -18.175      -25.071      -62.791      -19.029      -23.653
```

```
POINT ITN   T       CO         H2O        H2         N2         ZRO2(L)    PB         BI

  2    4 2664.85  -30.797     -37.224    -18.367    -25.271    -66.390    -18.457    -23.098

PHASE CHANGE, REPLACE ZRO2(L)       WITH ZRO2(B)
  2    2 2668.58  -30.795     -37.216    -18.372    -25.276    -66.784    -18.473    -23.106

PC/PT= 1.781106   T =  2668.58

POINT ITN   T       CO         H2O        H2         N2         ZRO2(B)    PB         BI

  2    3 2666.37  -30.801     -37.225    -18.374    -25.277    -66.738    -18.468     23.101

PC/PT= 1.789253   T =  2666.37
  2    2 2666.35  -30.801     -37.226    -18.374    -25.277    -66.738    -18.468    -23.101

PC/PT= 1.789311   T =  2666.35
  3    6 1894.37  -33.464     -41.961    -18.908    -25.867    -84.178    -15.823    -20.330

  3    4 1897.79  -33.448     -41.932    -18.906    -25.864    -84.867    -15.840    -20.349

  4    5 1713.91  -34.399     -43.699    -19.856    -26.842    -98.737    -14.803    -19.240

  4    3 1716.08  -34.387     -43.677    -19.854    -26.840    -90.653    -14.816    -19.254

  5    5 1567.74  -35.307     -45.418    -19.187    -26.204    -97.236    -13.783    -18.147

  5    3 1568.43  -35.302     -45.481    -19.186    -26.203    -97.203    -13.788    -18.153

  6    5 1496.82  -35.818     -46.365    -19.256    -26.291   -100.876    -13.209    -17.532

  6    3 1496.74  -35.811     -46.366    -19.256    -26.291   -100.880    -13.208    -17.531

  7    5 1404.05  -36.544     -47.764    -19.352    -26.416   -106.224    -12.362    -16.624

PHASE CHANGE, REPLACE ZRO2(B)       WITH ZRO2(A)
  7    2 1404.39  -36.542     -47.760    -19.353    -26.416   -106.229    -12.367    -16.629

POINT ITN   T       CO         H2O        H2         N2         ZRO2(A)    PB         BI

  7    3 1405.41  -36.533     -47.743    -19.352    -26.415   -106.166    -12.377    -16.640
```

THEORETICAL ROCKET PERFORMANCE ASSUMING EQUILIBRIUM COMPOSITION DURING EXPANSION

PC = 1480.0 PSIA
CASE NO. 30C

	CHEMICAL FORMULA				WT FRACTION (SEE NOTE)	ENERGY CAL/MOL	STATE	TEMP DEG K
FUEL	C 3.00000	O 9.00000	H 5.00000	N 3.00000	0.113600	-85300.000	S	298.15
FUEL	C 4.00000	O 9.00000	H 7.00000	N 3.00000	0.113600	-93070.000	S	298.15
FUEL	C 4.00000	O 8.00000	H 8.00000	N 8.00000	0.660000	17930.000	S	298.15
FUEL	C 10.00000	O 5.00000	H 16.00000		0.048300	-282900.000	S	298.15
FUEL	C 2.00000	O 1.00000	H 3.00000	N 1.00000	0.016800	-23550.000	S	298.15
FUEL	C 7.00000	O 2.00000	H 8.00000	N 2.00000	0.007500	-7460.000	S	298.15
FUEL	C 12.00000	O 2.00000	H 11.00000	N 2.00000	0.004000	-15400.000	S	298.15
FUEL	C 6.00000	O 7.00000	H 8.00000		0.003400	-655130.000	S	298.15
FUEL	C 12.00000	O 20.00000	H 15.00000	N 5.00000	0.003400	-160200.000	S	298.15
FUEL	ZR 1.00000	C 1.00000			0.010000	-48500.000	S	298.15
FUEL	PB 3.00000	C 12.00000	H 16.00000	O 17.00000	0.015000	0.000	S	298.15
FUEL	C 1.00000				0.004000	0.000	S	298.15
FUEL	BI 1.00000	C 18.00000	H 15.00000		0.000400	0.000	S	298.15

O/F= 0.0000 PERCENT FUEL= 100.0000 EQUIVALENCE RATIO= 1.6706 PHI= 0.0000

	CHAMBER	THROAT	EXIT	EXIT	EXIT	EXIT	EXIT
PC/P	1.0000	1.7893	10.525	17.458	27.340	34.519	47.384
P, ATM	100.71	56.283	9.5680	5.7711	3.6836	2.9174	2.1290
T, DEG K	2951.3	2666.4	1897.8	1716.0	1568.4	1496.7	1405.4
RHO, G/CC	9.9299-3	6.1562-3	1.4738-3	9.8254-4	6.8615-4	5.6947-4	4.4257-4
H, CAL/G	-134.63	-270.51	-603.48	-679.16	-748.24	-769.86	-807.74
U, CAL/G	-380.24	-491.92	-760.80	-821.43	-878.25	-893.92	-924.24
G, CAL/G	-7317.61	-6759.96	-5222.37	-4855.60	-4557.52	-4412.66	-4228.26
S, CAL/(G)(K)	2.4338	2.4338	2.4338	2.4338	2.4338	2.4338	2.4338
M, MOL WT	23.879	23.932	23.972	23.973	23.973	23.973	23.973
(DLV/DLP)T	-1.00287	-1.00091	-1.00004	-1.00002	-1.00001	-1.00001	-1.00001
(DLV/DLT)P	1.0422	1.0200	1.0008	1.0003	1.0001	1.0001	1.0001
CP, CAL/(G)(K)	0.5036	0.4638	0.4167	0.4131	0.4116	0.4114	0.4118
GAMMA (S)	1.2156	1.2275	1.2488	1.2512	1.2522	1.2524	1.2520
SON VEL,M/SEC	1117.7	1046.4	906.6	862.5	825.3	806.3	781.2
MACH NUMBER	0.000	1.000	2.185	2.474	2.728	2.859	3.038

PERFORMANCE PARAMETERS

AE/AT	1.0000	2.2500	3.1300	4.2500	5.0000	6.2500
CSTAR, FT/SEC	5100	5100	5100	5100	5100	5100
CF	0.686	1.274	1.373	1.448	1.483	1.527
IVAC,LB-SEC/LB	197.3	235.9	246.1	254.2	258.1	263.0
ISP, LB-SEC/LB	108.7	202.8	217.7	229.6	235.1	242.0

MOLE FRACTIONS

BI	2.1643-5	2.1691-5	2.1728-5	2.1729-5	2.1729-5	2.1729-5	2.1729-5
FORMALDEHYDE	2.4359-6	1.4218-6	3.0280-7	2.0095-7	1.4140-7	1.1834-7	9.3425-8
FORMIC ACID	2.5759-6	1.4072-6	2.3114-7	1.4134-7	9.2326-8	7.4299-8	5.5616-8
CH4	2.7273-8	2.3208-8	5.4614-8	1.6481-7	2.2171-7	3.4958-7	6.9219-7
CO	3.2199-1	3.1927-1	3.0317-1	2.9586-1	2.8811-1	2.8356-1	2.7685-1
CO2	7.0786-2	7.4379-2	9.1166-2	9.8488-2	1.0624-1	1.1079-1	1.1750-1
H	4.8998-3	2.4485-3	9.8475-5	2.8435-5	8.2388-6	4.1057-6	1.5159-6
HCN	6.5825-6	3.7915-6	7.9879-7	5.3192-7	3.7672-7	3.1667-7	2.5243-7
HCO RAD	1.2894-5	4.9660-6	1.2684-7	3.5457-8	1.0379-8	5.2783-9	2.8333-9
HNCO	1.6580-6	8.6723-7	1.1640-7	6.5166-8	3.8810-8	2.9607-8	2.0501-8
HNO	5.532 -7	1.130 -7	1.583-10	1.336-11	1.243-12	3.314-13	5.039-14
H2	1.3330-1	1.3712-1	1.5458-1	1.6193-1	1.6970-1	1.7424-1	1.8096-1

N2O	2.1628-1	2.0926-1	1.9404-1	1.8675-1	1.7908-1	1.7446-1	1.6775-1
N	5.822 -7	8.241 -8	3.876-11	1.584-12	8.420-14	1.635-14	1.573-15
NH	2.855 -6	4.757 -7	1.831 -9	1.895-10	1.189-11	3.472-12	6.033-13
NH2	2.790 -6	9.504 -7	1.486 -8	3.493 -9	8.645-10	4.088-10	1.355-10
NH3	1.8340-5	1.3390-5	7.2997-6	6.8513-6	6.7801-6	6.8627-6	7.1817-6
NO	3.326 -4	2.640 -5	3.633 -7	4.307 -8	5.162 -9	1.569 -9	2.857-10
N2	2.5239-1	2.5337-1	2.5356-1	2.5357-1	2.5357-1	2.5357-1	2.5357-1
O	5.657 -5	1.846 -5	4.837 -9	2.465-10	1.262-11	2.378-12	2.162-13
OH	2.5322-3	9.4698-4	1.0349-5	1.0187-6	3.3787-7	1.1941-7	2.9381-8
O2	3.580 -5	6.632 -6	2.652 -9	1.273-10	6.116-12	1.186-12	9.536-14
PB	9.4619-4	9.7666-4	1.0171-3	1.0196-3	1.0205-3	1.0208-3	1.0218-3
PBO	7.0855-5	4.2669-5	3.9989-6	1.6183-6	6.5349-7	3.9442-7	1.9191-7
ZRO2	9.487 -7	6.119 -8	2.769-13	2.475-15	2.253-17	1.686-18	3.577-20
ZRO2(A)	0.0000 0	0.0000 0	0.0000 0	0.0000 0	0.0000 0	0.0000 0	2.3169-3
ZRO2(B)	0.0000 0	2.3128-3	2.3168-3	2.3169-3	2.3169-3	2.3169-3	0.0000 0
ZRO2(L)	2.3068-3	0.0000 0	0.0000 0	0.0000 0	0.0000 0	0.0000 0	0.0000 0

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.50000E-06 FOR ALL ASSIGNED CONDITIONS

C	CH	CH2	CH3	HYDROXYMETHYLENE	METHYLOXIDE	METHANOL
CN	HCN RAD	CNN RAD	C2	C2H RAD	ACETYLENE	KETENE
C2H3 RAD	METHYL CYANIDE	CH3CO RAD	CH2CHO RAD	ETHYLENE	ACETALDEHYDE	ACETIC ACID
(FORMIC ACID)2	ETHYL RAD	ETHYL OXIDE RAD	ETHANE	AZOMETHANE	DIMETHYL ETHER	ETHANOL
CNC RAD	CYANOGEN	CCO RAD	C3	C3H3 RAD	CYCLOPROPENE	PROPYNE
ALLENE	C3H5 RAD	CYCLOPROPANE	PROPYLENE	PROPYLENE OXIDE	I-PROPYL RAD	N-PROPYL RAD
PROPANE	1-PROPANOL	CARBON SUBOXIDE	C4	BUTADIYNE	CYCLOBUTADIENE	BUTAN-1EN-3YN
1,3-BUTADIENE	2-BUTYNE	2-BUTENE TRANS	2-BUTENE CIS	ISOBUTENE	1-BUTENE	(ACETIC ACID)2
T-BUTYL RAD	S-BUTYL RAD	N-BUTYL RAD	N-BUTANE	ISOBUTANE	CARBON SUBNITRID	C5
CYCLOPENTADIENE	CYCLOPENTANE	1-PENTENE	T-PENTYL RAD	N-PENTYL RAD	PENTANE	ISOPENTANE
CH3C(CH3)2CH3	HEXATRIYNE	PHENYL RAD	PHENOXY RAD	BENZENE	PHENOL	CYCLOHEXENE
N-HEXYL RAD	TOLUENE	CRESOL	1-HEPTENE	N-HEPTYL RAD	N-HEPTANE	1-OCTENE
N-OCTYL RAD	OCTANE	ISO-OCTANE	N-NONYL RAD	NAPTHLENE	AZULENE	N-DECYL RAD
O-BIPHENYL RAD	BIPHENYL	JET-A(G)	HNO2	HNO3	NO2	N2H2
N2O2	NCO	NH2OH	NO2	NO3	N2H2	NH2NO2
N2H4	N2O	N2O3	N2O4	N2O5	N3	N3H
O3	PB2	ZR	ZRN	ZRO	BI(S)	BI(L)
C(GR)	BENZENE(L)	TOLUENE(L)	OCTANE(L)	JET-A(L)	H2O(S)	H2O(L)
PB(S)	PB(L)	PBO(RD)	PBO(YW)	PBO(L)	PBO2(S)	PB3O4(S)
ZR(A)	ZR(B)	ZR(L)	ZRN(S)	ZRN(L)		

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

THEORETICAL ROCKET PERFORMANCE ASSUMING FROZEN COMPOSITION DURING EXPANSION

PC = 1400.0 PSIA
CASE NO. 300

	CHEMICAL FORMULA				WT FRACTION (SEE NOTE)	ENERGY CAL/MOL	STATE	TEMP DEG K
FUEL	C 3.00000	O 9.00000	H 5.00000	N 3.00000	0.112600	-85300.000	S	298.15
FUEL	C 4.00000	O 9.00000	H 7.00000	N 3.00000	0.113600	-93870.000	S	298.15
FUEL	C 4.00000	O 8.00000	H 8.00000	N 8.00000	0.460000	17930.000	S	298.15
FUEL	C 10.00000	O 5.00000	H 16.00000		0.040300	-202900.000	S	298.15
FUEL	C 2.00000	O 1.00000	H 3.00000	N 1.00000	0.016803	-23550.000	S	298.15
FUEL	C 7.00000	O 2.00000	H 8.00000	N 2.00000	0.007500	-7460.000	S	298.15
FUEL	C 12.00000	O 2.00000	H 11.00000	N 2.00000	0.004000	-15400.000	S	298.15
FUEL	C 6.00000	O 7.00000	H 8.00000		0.003400	-655130.000	S	298.15
FUEL	C 12.00000	O 20.00000	H 15.00000	N 5.00000	0.003400	-160200.000	S	298.15
FUEL	ZR 1.00000	C 1.00000			0.010000	-48500.000	S	298.15
FUEL	PB 3.00000	C 12.00000	H 16.00000	O 17.00000	0.015000	0.000	S	298.15
FUEL	C 1.00000				0.004000	0.000	S	298.15
FUEL	BI 1.00000	C 18.00000	H 15.00000		0.000400	0.000	S	298.15

O/F= 0.0000 PERCENT FUEL= 100.0000 EQUIVALENCE RATIO= 1.6706 PHI= 0.0000

	CHAMBER	THROAT
PC/P	1.0000	
P, ATM	100.71	
T, DEG K	2951.3	
RHO, G/CC	9.9299-3	
H, CAL/G	-334.63	
U, CAL/G	-380.24	
G, CAL/G	-7317.61	
S, CAL/(G)(K)	2.4338	
M, MOL WT	23.879	
CP, CAL/(G)(K)	0.4273	
GAMMA (S)	1.2419	
SON VEL,M/SEC	1129.7	
MACH NUMBER	0.000	

PERFORMANCE PARAMETERS

AE/AT
CSTAR, FT/SEC
CF
IVAC,LB-SEC/LB
ISP, LB-SEC/LB

MOLE FRACTIONS

BI	0.00002	FORMALDEHYDE	0.00000	FORMIC ACID	0.00000	CO	0.32199
CO2	0.07079	H	0.00490	HCN	0.00001	HCO RAD	0.00001
HNCO	0.00000	HNO	0.00500	N2	0.13530	H2O	0.21628
N	0.00000	NH	0.00000	NH2	0.00000	NH3	0.00002
NO	0.00033	H2	0.25239	O	0.00006	OH	0.00253
O2	0.00004	PB	0.00095	PBO	0.00007	ZRO2	0.00000
ZRO2(L)	0.00331						

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.50000E-06 FOR ALL ASSIGNED CONDITIONS

C	CH	CH2	CH3	HYDROXYMETHYLENE	METHYLOXIDE	CH4
METHANOL	CN	HCN RAD	CNN RAD	C2	C2H RAD	ACETYLENE
KETENE	C2H3 RAD	METHYL CYANIDE	CH3CO RAD	CH2CHO RAD	ETHYLENE	ACETALDEHYDE
ACETIC ACID	(FORMIC ACID)2	ETHYL RAD	ETHYL OXIDE RAD	ETHANE	AZOMETHANE	DIMETHYL ETHER
ETHANOL	CNC RAD	CYANOGEN	CCO RAD	C3	C3H3 RAD	CYCLOPROPENE

PROPYNE	ALLENE	C3H5 RAD	CYCLOPROPANE	PROPYLENE	PROPYLENE OXIDE	I-PROPYL RAD
N-PROPYL RAD	PROPANE	1-PROPANOL	CARBON SUBOXIDE	C4	BUTADIYNE	CYCLOBUTADIENE
BUTAN-1EN-3YN	1,3-BUTADIENE	2-BUTYNE	2-BUTENE TRANS	2-BUTENE CIS	ISOBUTENE	1-BUTENE
(ACETIC ACID)2	T-BUTYL RAD	S-BUTYL RAD	N-BUTYL RAD	N-BUTANE	ISOBUTANE	CARBON SUBNITRID
C5	CYCLOPENTADIENE	CYCLOPENTANE	1-PENTENE	T-PENTYL RAD	N-PENTYL RAD	PENTANE
ISOPENTANE	CH3C(CH3)2CH3	HEXATRIYNE	PHENYL RAD	PHENOXY RAD	BENZENE	PHENOL
CYCLOHEXENE	N-HEXYL RAD	TOLUENE	CRESOL	1-HEPTENE	N-HEPTYL RAD	N-HEPTANE
1-OCTENE	N-OCTYL RAD	OCTANE	ISO-OCTANE	N-NONYL RAD	NAPTHLENE	AZULENE
N-DECYL RAD	O-BIPHENYL RAD	BIPHENYL	JET-A(G)	HNO2	HNO3	HO2
H2N2	H2O2	NCO	NH2OH	NO2	NO3	N2H2
NH2NO2	N2H4	N2O	N2O3	N2O4	N2O5	N3
N3H	O3	PB2	ZR	ZRN	ZRO	BI(S)
BI(L)	C(GR)	BENZENE(L)	TOLUENE(L)	OCTANE(L)	JET-A(L)	H2O(S)
H2O(L)	PB(S)	PB(L)	PBO(RD)	PBO(YW)	PBO(L)	PBO2(S)
PB3O4(S)	ZR(A)	ZR(B)	ZR(L)	ZRN(S)	ZRN(L)	ZRO2(A)
ZRO2(B)						

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

CALCULATIONS WERE STOPPED BECAUSE NEXT POINT IS MORE THAN 50 DEG BELOW TEMP RANGE OF A CONDENSED SPECIES

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