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CHEMICAL SPECIES *and* CHEMICAL REACTIONS  
*of importance in*  
 NONEQUILIBRIUM PERFORMANCE  
 CALCULATIONS

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*Prepared for*  
 NATIONAL AERONAUTICS AND SPACE ADMINISTRATION  
 MANNED SPACECRAFT CENTER  
*Under*  
 CONTRACT NAS9-4358

3.  
**TRW** SYSTEMS Group

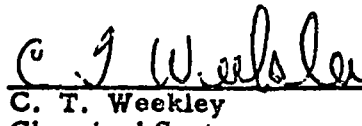
One Space Park • Redondo Beach, California

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OF IMPORTANCE IN  
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CALCULATIONS**

Prepared by:

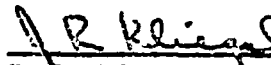


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## I. INTRODUCTION

This report contains the results of a study to determine the chemical species and chemical reactions of importance in nonequilibrium performance calculations. This study was performed by TRW Systems Group for NASA (MSC) under contract NAS 9-4358, Improvement of Analytical Predictions of Delivered Specific Impulse.

The objective of this contract was to develop a family of four computer programs to calculate inviscid, one-dimensional and axisymmetric non-equilibrium nozzle flow fields accounting for the nonequilibrium effects of finite rate chemical reactions between gaseous combustion products and velocity and thermal lags between gaseous and condensed combustion products.

The four programs developed under this contract are:

- A one-dimensional program which calculates the equilibrium, frozen and kinetic performance of propellant systems having gaseous exhaust products containing the elements carbon, hydrogen, oxygen, nitrogen, fluorine and chlorine.
- A one-dimensional program which calculates the equilibrium, frozen and kinetic performance of systems having gaseous and condensed exhaust products containing the elements carbon, hydrogen, oxygen, nitrogen, fluorine, chlorine and one metal element, either aluminum, beryllium, boron or lithium.
- An axisymmetric program which calculates the kinetic performance of propellant systems having gaseous exhaust products containing the elements carbon, hydrogen, oxygen, nitrogen, fluorine and chlorine. On option, this program considers either the expansion of a uniform mixture (the ideal engine case) or of a two-zoned mixture (the film cooled engine case).
- An axisymmetric program which calculates the kinetic performance of propellant systems having gaseous and condensed exhaust products containing the elements carbon, hydrogen, oxygen, nitrogen, fluorine, chlorine and one metal element, either aluminum, beryllium, boron or lithium. This program considers only the expansion of a uniform mixture (the ideal engine case).

These programs differ in a number of ways from previous programs developed to calculate nonequilibrium nozzle expansions.

**In particular:**

- The programs are completely self-contained requiring specification of only the propellant system (elemental composition and heat of formation), relaxation rates and nozzle geometry to run a case.
- The chemical species considered by the programs have been selected to allow accurate equilibrium, frozen and kinetic performance analyses of cryogenic, space storable, pre-packaged, hybrid and solid propellant systems of current and projected operational use.
- All dissociation-recombination and binary exchange reactions between the gaseous species present in the exhaust are considered by the programs allowing complete kinetic expansion calculations.
- The programs utilize TRW Systems implicit integration method which allows rapid integration of the chemical and gas-particle relaxation equations from equilibrium chamber conditions. Typical run times are three minutes for the one-dimensional programs and ten minutes for the axisymmetric programs on an IBM 7094 Mod II computer.
- The programs allow analysis of the performance loss associated with film cooling in propellant systems having all gaseous exhaust products.
- The programs allow simultaneous consideration of both chemical and gas-particle relaxation losses in propellant systems having condensed exhaust products.
- The one-dimensional programs allow equilibrium, frozen and kinetic performance calculations to be performed during a single machine run.
- The programs are written in machine independent language (Fortran IV) allowing their use on all standard computers.

The study described in this report was performed to determine the significant chemical species and chemical reactions which need be considered in nonequilibrium performance calculations for typical propellant systems containing the elements: carbon, hydrogen, oxygen, nitrogen, fluorine, chlorine; and one metal element, either aluminum, beryllium, boron or lithium. The significant chemical species were defined in contract NAS 9-4358 as those which must be considered to determine the equilibrium of the propellant systems under investigation to within 0.5 second of specific impulse at an area ratio of 40. The selection

of the significant chemical species in typical propellant exhaust mixtures on the basis of equilibrium performance calculations does not, however, insure the validity of the selection for all nonequilibrium performance calculations. If the significant chemical species selection is valid for both equilibrium flow (infinite reaction rates) and frozen flow (zero reaction rates), however, the selection will also be valid for nonequilibrium flows having finite reaction rates. Thus, an additional restriction was imposed on the significant chemical species selection and the significant chemical species were defined as those which must be considered to determine both the equilibrium and frozen specific impulse of the propellant systems under investigation to within 0.5 second at an area ratio of 40.

After determining the significant species, all possible dissociation-recombination and binary exchange reactions between these species were studied. Those reactions having an energy barrier due to the fact that they cannot occur in the ground state (the so-called "spin forbidden" reactions) were identified, and those reactions, which while stoichiometrically possible were highly improbable due to structural or steric factors, were identified and eliminated from consideration. A literature rate survey was performed to determine the status of rate data for the chemical reactions of interest.

These studies are described in the following sections.

## 2. CHEMICAL SPECIES STUDY

A number of propellant systems containing the elements: carbon, hydrogen, oxygen, nitrogen, fluorine and chlorine, and one metal element, either aluminum, beryllium, boron or lithium, were selected as representative of typical liquid rocket cryogenic, space storable and prepackaged storable propellant systems, hybrid and solid rocket propellants. The propellant systems selected for study are given in Table I of Appendix A. These propellant systems are representative of current and projected operational propellant systems.

The number of chemical species in the exhaust mixtures of these propellants for which JANAF thermochemical data exists is over one hundred. The number of chemical reactions between these species which are stoichiometrically possible is naturally immense. It is clearly undesirable

to attempt to account for all possible chemical species and chemical reactions in nonequilibrium performance calculations since it is known that relatively few of the total possible species and reactions are of engineering importance in nozzle and plume expansions.

The approach taken in this study to determine the minimum number of species which must be considered in nonequilibrium performance calculations was to consider equilibrium and frozen expansions as the limits of nonequilibrium expansions. Thus, by determining the significant species which must be considered to accurately calculate the equilibrium and frozen performance of these typical propellant systems, the significant species which must be considered in calculating the nonequilibrium performance of these and similar propellant systems can be determined. For the purpose of this study, the significant chemical species were thus defined as those which must be considered to determine both the equilibrium and frozen specific impulse of the propellant systems considered in the study to within 0.5 second at an area ratio of 40.

Equilibrium and frozen performance calculations were performed for the propellant systems listed in Table I, Appendix A, at two chamber pressures, 100 psia and 1000 psia, considering all species for which JANAF thermochemical data exist present in the exhaust mixtures. These calculations were used as the reference calculations for comparison with calculations performed considering fewer species. Those molecular species appearing in only trace amounts (less than approximately  $10^{-3}$  mole percent) in the reference calculations were neglected and the calculations repeated to determine the effect of neglecting trace species on the calculated equilibrium and frozen performance of these propellant systems. After a series of such calculations considering different chemical species present in the various exhaust mixtures, it was determined that the significant species present in these exhaust mixtures are those given in Table II, Appendix A. Those significant species present in each propellant system studied are given in Table III, Appendix A. Comparisons of the equilibrium and frozen performance calculated considering all species present and only the significant species present is given in Tables IV through XXXVII in Appendix A for all propellant systems studied.

Examination of Tables IV through XXXVII, Appendix A, shows that for the nonmetallized propellant systems the maximum performance difference between the calculations considering all species present and only the significant species present is 0.49 second of specific impulse at an area ratio of 40. This difference occurs in the frozen performance calculation of the Chlorine Trifluoride/86% Monomethyl Hydrazine + 14% Hydrazine system at a mixture ratio of 3.2 and 100 psia chamber pressure. In the metallized systems, the maximum performance difference is 0.38 second of specific impulse at an area ratio of 40 which occurs in the frozen performance calculation of the double base-beryllium-ammonium perchlorate system for 100 psia chamber pressure. It is seen that the neglected chemical species have little effect on the calculated performance of the propellant systems studied. Thus, performance calculations performed considering only the significant chemical species given in Table II present in the exhaust mixture will allow the accurate determination of the equilibrium, frozen and non-equilibrium performance of these and similar propellant systems.

Although the significant chemical species given in Table II were determined from studying specific propellant systems, the utility of nonequilibrium performance programs based on this species selection is not limited to these specific propellant systems, but is equally valid for chemically similar propellant systems. In studying similar propellant systems, the applicability of the significant species selection can be simply established by comparing equilibrium and frozen performance calculations considering all species present and only the significant species present. For chemically nonsimilar systems, the above methods can be readily utilized to determine the significant chemical species in these systems.

### 3. CHEMICAL REACTION STUDY

Having identified the significant chemical species in the above propellant systems, all possible recombination-dissociation and binary exchange reactions between the significant species present in each propellant system were studied. Those reactions which, although stoichiometrically possible, were highly improbable on the basis of structural or steric factors were eliminated resulting in the identification of those reactions given in Tables I through VI, Appendix B, as those reactions of possible chemical significance



in nonequilibrium expansions of the propellant systems studied.

Those reactions eliminated due to steric and structural arguments (listed in Table VII, Appendix B) involve the breaking and formation of a number of chemical bonds and molecular rearrangements which are highly improbable compared to other reactions which can occur between the same species.

Although arguments can be given that some of the reactions identified to be of possible chemical significance in the nonequilibrium expansion of the propellant systems studied can be of little significance due to concentration considerations or possible activation energy considerations, current lack of rate knowledge precludes their elimination at this time. This approach of retaining all possible chemical reactions in nonequilibrium calculations which cannot be eliminated due to steric consideration insures that future rate measurements which may change the relative importance of various chemical reactions will not affect the nonequilibrium computer programs developed by TRW for NASA.

#### 4. CHEMICAL REACTION RATE STUDY

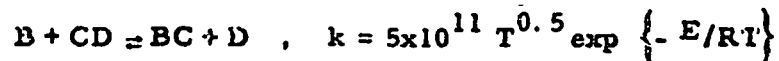
A literature survey was performed to determine the status of rate data for the chemical reactions given in Tables I through VI of Appendix B. Those reactions for which rates have been reported are given in Table IX of Appendix B. In addition, those reactions having an energy barrier due to the fact that they cannot occur in the ground state (the so-called "spin forbidden" reactions) were identified and are listed in Table VIII of Appendix B.

Order of magnitude rate estimates can be obtained by statistical mechanics and kinetic theory for those reactions for which rate data are not reported. When rate constants are represented by an Arrhenius equation,  $k = AT^n \exp(-E/RT)$ , where  $T$  is the absolute temperature,  $R$  is the gas constant,  $A$  is the frequency factor,  $E$  is the activation energy, and  $n$  determines the pre-exponential temperature dependence, order of magnitude approximations can be made as follows:

##### A. Exothermic, trimolecular reactions

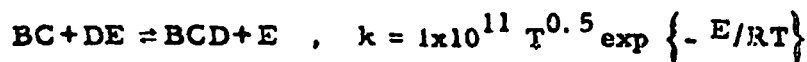


B. Exothermic, bimolecular reactions with triatomic transition states.



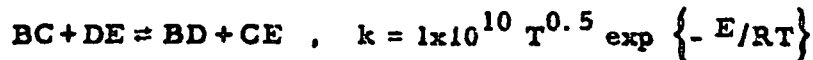
where  $E = 5.5\%$  of the CD bond energy (Hirschfelder Rule)

C. Exothermic, bimolecular reactions with transition states of more than three atoms



where  $E = 5.5\%$  of the DE bond energy

D. Exothermic, bimolecular, binary exchange reactions



where  $E = 28\%$  of the sum of the BC and DE bond energies

The reaction rates for the "spin forbidden" reactions can be similarly estimated if the rate constants are corrected by Boltzmann factors for the fact that these reactions do not occur in the ground state.

The above methods of estimating exothermic reaction rates are similar to those used by Tunder, et al. \*

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\* R. Tunder, S. Mayer, B. Cook, and L. Schieler, "Compilation of Reaction Rate Data for Nonequilibrium Performance and Re-entry Calculation Programs," Aerospace Corporation (1966).

APPENDIX A

Table I. Propellant Systems Studied at Chamber Pressures of 100 and 1000 psia to Identify Significant Chemical Species

<u>Oxidizer/Fuel</u>	<u>Mixture Ratios</u>
1. Oxygen/Hydrogen	MR = 2.0, 4.0, 5.0, 6.0, 10.0
2. Fluorine/Hydrogen	MR = 3.0, 7.0, 10.0, 13.0, 20.0
3. Oxygen/RP-1	MR = 1.0, 2.2, 2.6, 3.0, 5.0
4. Nitrogen Tetroxide/Hydrazine	MR = 0.5, 0.9, 1.1, 1.3, 2.0
5. Compound "A"/ Hydrazine	MR = 1.0, 2.3, 2.5, 2.7, 5.0
6. Nitrogen Tetroxide/Monomethyl Hydrazine	MR = 0.5, 1.5, 1.8, 2.1, 3.5
7. Oxygen Difluoride/Monomethyl Hydrazine	MR = 0.5, 1.5, 1.8, 2.1, 3.5
8. Perchloryl Fluoride/Monomethyl Hydrazine	MR = 0.5, 1.5, 1.8, 2.1, 3.5
9. Hydrazine/Diborane	MR = 1.15, 1.25, 1.35
10. Oxygen Difluoride/Diborane	MR = 2.4, 3.2, 4.0
11. Oxygen Difluoride/Lithium Hydride	MR = 2.5, 3.0, 3.5
12. Chlorine Trifluoride/86% Monomethyl Hydrazine+14% Hydrazine	MR = 2.4, 2.8, 3.2
13. Chlorine Trifluoride/49% Monomethyl Hydrazine+8% Hydrazine+ 43% Aluminum	MR = 2.5, 3.0, 3.5
14. Chlorine Trifluoride/43% Monomethyl Hydrazine+7% Hydrazine+ 50% Boron	MR = 4.0, 5.0, 6.0
15. Chlorine Trifluoride/43% Monomethyl Hydrazine+7% Hydrazine+ 50% Beryllium	MR = 3.5, 4.5, 5.5

Table 1 (Continued)

<u>Oxidizer/Fuel</u>	<u>Composition</u>	
16. Ammonium Perchlorate/PBAA— Aluminum	14 percent Organic Fuel	
	16 "	Aluminum
	70 "	$\text{NH}_4\text{ClO}_4$
17. Ammonium Perchlorate/PBAA— Beryllium	16 "	Organic Fuel
	13 "	Beryllium
	71 "	$\text{NH}_4\text{ClO}_4$
18. Ammonium Perchlorate/Double Base— Aluminum	69.4 "	Double Base
	19.8 "	Aluminum
	10.8 "	$\text{NH}_4\text{ClO}_4$
19. Ammonium Perchlorate/Double Base— Beryllium	81 "	Double Base
	10 "	Beryllium
	9 "	$\text{NH}_4\text{ClO}_4$

Table II. Species Selected for Use in the TRW/NASA Nonequilibrium Performance Programs

Basic Species for C, H, N, O, Cl, and F Propellant Systems Having Gaseous Combustion Products

C	Cl	F	H	N	O
CO	Cl <sub>2</sub>	F <sub>2</sub>	H <sub>2</sub>	N <sub>2</sub>	O <sub>2</sub>
CO <sub>2</sub>	ClF		H <sub>2</sub> O	NO	OH
			HF		
			HCl		

Additional Species for Propellant Systems Having Condensed Carbon as a Combustion Product

Additional Species for Propellant Systems Containing Aluminum

Additional Species for Propellant Systems Containing Boron

Additional Species for Propellant Systems Containing Beryllium

Additional Species for Propellant Systems Containing Lithium

C(S)	Al	B	Be	Li
C <sub>2</sub>	AlO	B(L)	BeOH	LiH
CH	Al <sub>2</sub> O	B(S)	BeO <sub>2</sub> H <sub>2</sub>	LiOH
CH <sub>2</sub>	Al <sub>2</sub> O <sub>3</sub> (L)	BO	BeO	LiO
CH <sub>3</sub>	Al <sub>2</sub> O <sub>3</sub> (S)	BO <sub>2</sub>	BeC(L)	Li <sub>2</sub> O
CH <sub>4</sub>	AlOCl	BF	BeC(S)	LiCl
C <sub>2</sub> H <sub>2</sub>	AlOF	BF <sub>2</sub>	Be <sub>2</sub> O	LiF
CF	AlCl	BF <sub>3</sub>	BeCl	Li <sub>2</sub> F <sub>2</sub>
C <sub>2</sub> F <sub>2</sub>	AlCl <sub>2</sub>	BCl	BeCl <sub>2</sub>	
CN	AlCl <sub>3</sub>	BCl <sub>2</sub>	BeF	
CiCN	AlClF	BCl <sub>3</sub>	BeF <sub>2</sub>	
FCN	AlClF <sub>2</sub>	BClF	BeClF	
HCN	AlCl <sub>2</sub> F	BCl <sub>2</sub> F		
	AlF	BClF <sub>2</sub>		
	AlF <sub>2</sub>	BOF		
	AlF <sub>3</sub>	BOCl		
		BN		
		BN(S)		

**Table III. Significant Species Considered in Each Propellant System**

Propellant System (Table I)

$O_2/H_2$	$F_2/H_2$	$O_7/RP-1$	$N_2O_4/H_2H_4$	$A/N_2H_4$
Species				
H	H	C	H	Cl
$H_2$	$H_2$	C(S)	$H_2$	$Cl_2$
$H_2O$	HF	CO	$H_2O$	ClF
O	F	$CO_2$	N	F
$O_2$	$F_2$	$C_2$	$N_2$	$F_2$
OH		CH	NO	H
		$CH_2$	O	$H_2$
		$CH_3$	$O_2$	HF
		$CH_4$	OH	HCl
		$C_2H_2$		N
		H		$N_2$
		$H_2$		
		$H_2O$		
		O		
		$O_2$		
		OH		
Total Number of Species Considered In Each Case				
6	5	15	9	11

Table III. (Continued)  
Propellant System

$N_2O_4/MMH$	$OF_2/MMH$	$ClO_3F/MMH$	$N_2H_4/B_2H_6$	$OF_2/B_2H_6$
		Species		
C	C	C	B	B
C(S)	C(S)	C(S)	B(L)	B(L)
CO	CO	CO	B(S)	B(S)
CO <sub>2</sub>	CO <sub>2</sub>	CO <sub>2</sub>	BN	BO
CN	CN	CN	BN(S)	BO <sub>2</sub>
C <sub>2</sub>	C <sub>2</sub>	C <sub>2</sub>	H	BF
CH	CH	CH	H <sub>2</sub>	BF <sub>2</sub>
CH <sub>2</sub>	CH <sub>2</sub>	CH <sub>2</sub>	N	BF <sub>3</sub>
CH <sub>3</sub>	CH <sub>3</sub>	CH <sub>3</sub>	N <sub>2</sub>	BOF
CH <sub>4</sub>	CH <sub>4</sub>	CH <sub>4</sub>		F
C <sub>2</sub> H <sub>2</sub>	C <sub>2</sub> H <sub>2</sub>	C <sub>2</sub> H <sub>2</sub>		F <sub>2</sub>
H	CF	CF		H
H <sub>2</sub>	C <sub>2</sub> F <sub>2</sub>	C <sub>2</sub> F <sub>2</sub>		H <sub>2</sub>
H <sub>2</sub> O	F	Cl		H <sub>2</sub> O
HCN	F <sub>2</sub>	Cl <sub>2</sub>		HF
N	FCN	ClCN		O
N <sub>2</sub>	H	ClF		C <sub>2</sub>
NO	H <sub>2</sub>	F		OH
O	H <sub>2</sub> O	F <sub>2</sub>		
O <sub>2</sub>	HF	FCN		
OH	HCN	H		
	N	H <sub>2</sub>		
	N <sub>2</sub>	H <sub>2</sub> O		
	NO	HF		
	O	HCl		
	O <sub>2</sub>	HCN		
	OH	N		
		N <sub>2</sub>		
		NO		
		O		
		O <sub>2</sub>		
		OH		
Total Number of Species Considered in Each System				
21	27	32	9	18



Table III. (Continued)  
Propellant System

OF <sub>2</sub> /H <sub>2</sub> O	CF/80% MMH 14% N <sub>2</sub> H <sub>4</sub>	CF/	CF/	CF/
		49% AlH <sub>3</sub> 8% N <sub>2</sub> H <sub>4</sub> 43% Al	44% MMH 7% N <sub>2</sub> H <sub>4</sub> 50% B	44% MMH 7% N <sub>2</sub> H <sub>4</sub> 50% B
Species				
F	C	C	C	C
F <sub>2</sub>	C(N)	C(N)	C(N)	C(N)
H	C <sub>2</sub>	C <sub>2</sub>	C <sub>2</sub>	C <sub>2</sub>
H <sub>2</sub>	CN	CN	CN	CN
H <sub>2</sub> O	CH	CH	CH	CH
HF	CH <sub>2</sub>	CH <sub>2</sub>	CH <sub>2</sub>	CH <sub>2</sub>
Li	CH <sub>3</sub>	CH <sub>3</sub>	CH <sub>3</sub>	CH <sub>3</sub>
LiH	CH <sub>4</sub>	CH <sub>4</sub>	CH <sub>4</sub>	CH <sub>4</sub>
LiOH	C <sub>2</sub> H <sub>2</sub>	C <sub>2</sub> H <sub>2</sub>	C <sub>2</sub> H <sub>2</sub>	C <sub>2</sub> H <sub>2</sub>
LiO	CF	CF	CF	CF
Li <sub>2</sub> O	C <sub>2</sub> F <sub>2</sub>	C <sub>2</sub> F <sub>2</sub>	C <sub>2</sub> F <sub>2</sub>	C <sub>2</sub> F <sub>2</sub>
HCl	Cl	Cl	Cl	Cl
H <sub>2</sub> F <sub>2</sub>	Cl <sub>2</sub>	Cl <sub>2</sub>	Cl <sub>2</sub>	Cl <sub>2</sub>
O	CICN	CICN	CICN	CICN
O <sub>2</sub>	CIF	CIF	CIF	CIF
OH	F	F	F	F
	F <sub>2</sub>	F <sub>2</sub>	F <sub>2</sub>	F <sub>2</sub>
	FCN	FCN	FCN	FCN
	H	H	H	H
	H <sub>2</sub>	H <sub>2</sub>	H <sub>2</sub>	H <sub>2</sub>
	HF	HF	HF	HF
	HCl	HCl	HCl	HCl
	HCN	HCN	HCN	HCN
	N	N	N	N
	N <sub>2</sub>	N <sub>2</sub>	N <sub>2</sub>	N <sub>2</sub>
		Al	B	Be
		AlCl	B(L)	BeCl
		AlCl <sub>2</sub>	B(S)	BeCl <sub>2</sub>
		AlF	BF	BeF
		AlF <sub>2</sub>	BF <sub>2</sub>	BeF <sub>2</sub>
		AlF <sub>3</sub>	BF <sub>3</sub>	BeClF
		AlCl <sub>3</sub>	BN	
		AlClF	BN(S)	
		AlClF <sub>2</sub>	BCl	
		AlCl <sub>2</sub> F	BCl <sub>2</sub>	
			BCl <sub>3</sub>	
			BClF	
			BCl <sub>2</sub> F	
			BClF <sub>2</sub>	

Total Number of  
Species Considered  
In Each System

Table III. (Continued)  
Propellant System

AP/PDAA-Al	AP/PBAA-Be	AP/DB-Al	AP/DB-Be
Species			
C	C	C	C
C(S)	C(S)	C(S)	C(S)
CO	CO	CO	CO
CO <sub>2</sub>	CO <sub>2</sub>	CO <sub>2</sub>	CO <sub>2</sub>
CN	CN	CN	CN
C <sub>2</sub>	C <sub>2</sub>	C <sub>2</sub>	C <sub>2</sub>
CH	CH	CH	CH
CH <sub>2</sub>	CH <sub>2</sub>	CH <sub>2</sub>	CH <sub>2</sub>
CH <sub>3</sub>	CH <sub>3</sub>	CH <sub>3</sub>	CH <sub>3</sub>
CH <sub>4</sub>	CH <sub>4</sub>	CH <sub>4</sub>	CH <sub>4</sub>
C <sub>2</sub> H <sub>2</sub>	C <sub>2</sub> H <sub>2</sub>	C <sub>2</sub> H <sub>2</sub>	C <sub>2</sub> H <sub>2</sub>
Cl	Cl	Cl	Cl
Cl <sub>2</sub>	Cl <sub>2</sub>	Cl <sub>2</sub>	Cl <sub>2</sub>
ClCN	ClCN	ClCN	ClCN
H	H	H	H
H <sub>2</sub>	H <sub>2</sub>	H <sub>2</sub>	H <sub>2</sub>
H <sub>2</sub> O	H <sub>2</sub> O	H <sub>2</sub> O	H <sub>2</sub> O
HCl	HCl	HCl	HCl
HCN	HCN	HCN	HCN
N	N	N	N
N <sub>2</sub>	N <sub>2</sub>	N <sub>2</sub>	N <sub>2</sub>
NO	NO	NO	NO
O	O	O	O
O <sub>2</sub>	O <sub>2</sub>	O <sub>2</sub>	O <sub>2</sub>
OH	OH	OH	OH
Al	Be	Al	Be
AlO	BeOH	AlO	BeOH
Al <sub>2</sub> O	BeO <sub>2</sub> H <sub>2</sub>	Al <sub>2</sub> O	BeO <sub>2</sub> H <sub>2</sub>
Al <sub>2</sub> O <sub>3</sub> (L)	BeO	Al <sub>2</sub> O <sub>3</sub> (L)	BeO
Al <sub>2</sub> O <sub>3</sub> (S)	BeO(L)	Al <sub>2</sub> O <sub>3</sub> (S)	BeO(L)
AlCl	BeO(S)	AlCl	BeO(S)
AlCl <sub>2</sub>	BeCl	AlCl <sub>2</sub>	BeCl
AlOCl	BeCl <sub>2</sub>	AlOCl	BeCl <sub>2</sub>
AlCl <sub>3</sub>	Be <sub>2</sub> O	AlCl <sub>3</sub>	Be <sub>2</sub> O
Total Number of Species Considered In Each System			
34	34	34	34

Table IV. Theoretical Specific Impulse of O<sub>2</sub>/H<sub>2</sub> System  
Chamber Pressure = 100 psia

Mixture Ratio	Area Ratio	Equilibrium Flow			Frozen Flow		
		All Species	6 Significant Species	$\Delta I_{sp}$	All Species	6 Significant Species	$\Delta I_{sp}$
2.0	10.0	406.89	406.88	0.01	406.77	406.78	0.01
	20.0	419.36	419.36	0.00	419.25	419.25	0.00
	30.0	425.18	425.18	0.00	425.06	425.06	0.00
	40.0	428.76	428.76	0.00	428.64	428.65	0.01
4.0	10.0	425.99	425.99	0.00	415.04	415.04	0.00
	20.0	442.84	442.84	0.00	430.36	430.36	0.00
	30.0	450.70	450.70	0.00	437.48	437.48	0.00
	40.0	455.55	455.55	0.00	441.87	441.87	0.00
5.0	10.0	421.42	421.42	0.00	402.37	402.37	0.00
	20.0	440.51	440.51	0.00	418.04	418.04	0.00
	30.0	449.67	449.67	0.00	425.39	425.39	0.00
	40.0	455.40	455.40	0.00	429.93	429.93	0.00
6.0	10.0	412.08	412.08	0.00	387.58	387.58	0.00
	20.0	433.09	433.09	0.00	403.10	403.10	0.00
	30.0	443.41	443.41	0.00	410.43	410.43	0.00
	40.0	449.98	449.98	0.00	414.97	414.98	0.01
10.0	10.0	359.60	359.61	0.01	336.24	336.24	0.00
	20.0	379.67	379.68	0.01	349.97	349.97	0.00
	30.0	389.92	389.93	0.01	356.48	356.49	0.01
	40.0	396.60	396.60	0.00	360.54	360.55	0.01

Table V. Theoretical Specific Impulse of O<sub>2</sub>/H<sub>2</sub> System  
 Chamber Pressure = 1000 psia

Mixture Ratio	Area Ratio	Equilibrium Flow			Frozen Flow		
		All Species	6 Significant Species	$\Delta I_{sp}$	All Species	Significant Species	$\Delta I_{sp}$
2.0	10.0	406.89	406.87	0.02	406.85	406.85	0.00
	20.0	419.36	419.36	0.00	419.32	419.32	0.00
	30.0	425.18	425.18	0.00	425.14	425.14	0.00
	40.0	428.76	428.76	0.00	428.72	428.73	0.01
4.0	10.0	427.01	427.01	0.00	422.02	422.02	0.00
	20.0	443.60	443.60	0.00	437.95	437.95	0.00
	30.0	451.35	451.35	0.00	445.37	445.37	0.00
	40.0	456.13	456.13	0.00	449.95	449.95	0.00
5.0	10.0	424.36	424.36	0.00	413.55	413.55	0.00
	20.0	442.80	442.81	0.01	430.25	430.25	0.00
	30.0	451.66	451.66	0.00	438.15	438.15	0.00
	40.0	457.19	457.19	0.00	443.06	443.06	0.00
6.0	10.0	417.72	417.72	0.00	401.19	401.19	0.00
	20.0	437.68	437.68	0.00	417.96	417.97	0.01
	30.0	447.46	447.46	0.00	425.99	426.00	0.01
	40.0	453.68	453.68	0.00	431.01	431.02	0.01
10.0	10.0	366.60	366.61	0.01	348.49	348.52	0.03
	20.0	386.06	386.08	0.02	363.34	363.38	0.04
	30.0	395.86	395.87	0.01	370.50	370.53	0.03
	40.0	402.19	402.20	0.01	374.99	375.02	0.03

Table VI. Theoretical Performance of F<sub>2</sub>/H<sub>2</sub> System  
 Chamber Pressure = 100 psia

Mixture Ratio	Area Ratio	Equilibrium Flow			Frozen Flow		
		All Species	5 Significant Species	$\Delta I_{sp}$	All Species	5 Significant Species	$\Delta I_{sp}$
3.0	10.0	425.46	425.46	0.00	423.31	423.31	0.00
	20.0	437.38	437.38	0.00	435.12	435.13	0.01
	30.0	442.97	442.88	0.01	440.57	440.57	0.00
	40.0	446.26	446.26	0.00	443.91	443.91	0.00
7.0	10.0	443.93	443.93	0.00	410.45	410.49	0.00
	20.0	460.76	460.76	0.00	421.97	421.97	0.00
	30.0	468.33	468.33	0.00	427.10	427.10	0.00
	40.0	472.87	472.87	0.00	430.22	430.22	0.00
10.0	10.0	439.15	439.15	0.00	397.12	397.12	0.00
	20.0	458.94	458.94	0.00	407.91	407.91	0.00
	30.0	468.23	468.23	0.00	412.68	412.68	0.00
	40.0	473.92	473.92	0.00	415.56	415.56	0.00
13.0	10.0	433.94	433.94	0.00	387.44	387.44	0.00
	20.0	454.89	454.89	0.00	397.75	397.75	0.00
	30.0	465.13	465.13	0.00	402.28	402.28	0.00
	40.0	471.57	471.57	0.00	405.00	405.00	0.00
20.0	10.0	416.55	416.56	0.01	363.45	363.45	0.00
	20.0	438.62	438.63	0.01	372.74	372.74	0.00
	30.0	449.49	449.49	0.00	376.81	376.81	0.00
	40.0	456.23	456.24	0.01	379.24	379.25	0.01

Table VII. Theoretical Performance of F<sub>2</sub>/H<sub>2</sub> System  
 Chamber Pressure = 1000 psia

Mixture Ratio	Area Ratio	Equilibrium Flow			Frozen Flow		
		All Species	5 Significant Species	$\Delta I_{sp}$	All Species	5 Significant Species	$\Delta I_{sp}$
3.0	10.0	425.51	425.51	0.00	424.77	424.77	0.00
	20.0	437.42	437.42	0.00	436.64	436.64	0.00
	30.0	442.91	442.91	0.00	442.12	442.12	0.00
	40.0	446.28	446.28	0.00	445.48	445.48	0.00
7.0	10.0	448.06	448.06	0.00	426.87	426.87	0.00
	20.0	463.74	463.74	0.00	439.46	439.46	0.00
	30.0	470.78	470.78	0.00	445.06	445.06	0.00
	40.0	475.01	475.01	0.00	448.45	448.45	0.00
10.0	10.0	447.25	447.25	0.00	416.27	416.27	0.00
	20.0	465.21	465.21	0.00	423.40	428.40	0.00
	30.0	473.51	473.51	0.00	433.75	433.76	0.01
	40.0	478.57	478.57	0.00	436.97	436.97	0.00
13.0	10.0	444.18	444.18	0.00	407.19	407.19	0.00
	20.0	463.58	463.58	0.00	418.88	418.88	0.00
	30.0	472.74	472.74	0.00	424.01	424.02	0.01
	40.0	478.41	478.41	0.00	427.08	427.10	0.02
20.0	10.0	428.82	428.82	0.00	383.44	383.44	0.00
	20.0	449.06	449.07	0.01	393.98	393.99	0.01
	30.0	458.41	458.42	0.01	398.59	398.59	0.00
	40.0	464.16	464.16	0.00	401.34	401.33	0.01

Table VIII. Theoretical Performance of O<sub>2</sub>/RP-1 System  
 Chamber Pressure = 100 psia

Mixture Ratio	Area Ratio	Equilibrium Flow			Frozen Flow		
		All Species	16 Significant Species	$\Delta I_{sp}$	All Species	16 Significant Species	$\Delta I_{sp}$
1.0	10.0	243.42	243.42	0.00	225.54	225.54	0.00
	20.0	256.28	256.28	0.00	232.46	232.46	0.00
	30.0	263.00	263.01	0.01	235.62	235.62	0.00
	40.0	267.48	267.48	0.00	237.51	237.51	0.00
2.2	10.0	320.10	320.10	0.00	301.61	301.62	0.01
	20.0	335.14	335.14	0.00	313.17	313.18	0.01
	30.0	342.49	342.49	0.00	318.61	318.62	0.01
	40.0	347.17	347.17	0.00	321.98	321.99	0.01
2.6	10.0	320.65	320.65	0.00	297.29	297.30	0.01
	20.0	338.29	338.29	0.00	309.03	309.04	0.01
	30.0	347.17	347.18	0.01	314.60	314.60	0.00
	40.0	352.91	352.91	0.00	318.06	318.07	0.01
3.0	10.0	315.06	315.07	0.01	291.40	291.40	0.00
	20.0	333.32	333.32	0.00	303.08	303.08	0.00
	30.0	342.84	342.84	0.00	308.65	308.65	0.00
	40.0	349.15	349.16	0.01	312.11	312.12	0.01
5.0	10.0	286.97	286.97	0.00	266.60	266.61	0.01
	20.0	303.36	303.37	0.01	277.51	277.53	0.02
	30.0	311.83	311.84	0.01	282.74	282.76	0.02
	40.0	317.40	317.41	0.01	286.03	286.03	0.00

Table IX. Theoretical Performance of O<sub>2</sub>/RP-1 System  
 Chamber Pressure = 1000 psia

Mixture Ratio	Area Ratio	Equilibrium Flow			Frozen Flow		
		All Species	16 Significant Species	$\Delta I_{sp}$	All Species	16 Significant Species	$\Delta I_{sp}$
1.0	10.0	250.41	250.42	0.01	232.73	232.74	0.01
	20.0	263.46	263.46	0.00	240.11	240.12	0.01
	30.0	270.24	270.24	0.00	243.52	243.53	0.01
	40.0	274.74	274.74	0.00	245.61	245.62	0.01
2.2	10.0	323.22	323.22	0.00	311.55	311.57	0.02
	20.0	337.63	337.63	0.00	323.94	323.96	0.02
	30.0	344.68	344.69	0.01	329.83	329.85	0.02
	40.0	349.18	349.18	0.00	333.49	333.52	0.03
2.6	10.0	327.31	327.32	0.01	309.12	309.14	0.02
	20.0	344.08	344.09	0.01	321.85	321.88	0.03
	30.0	352.41	352.41	0.00	327.97	328.00	0.03
	40.0	357.75	357.76	0.01	331.82	331.84	0.02
3.0	10.0	323.21	323.22	0.01	303.46	303.48	0.02
	20.0	341.38	341.39	0.01	316.16	316.18	0.02
	30.0	350.77	350.77	0.00	322.29	322.32	0.03
	40.0	356.94	356.94	0.00	326.16	326.18	0.02
5.0	10.0	293.24	293.25	0.01	276.55	276.58	0.03
	20.0	309.32	309.33	0.01	288.31	288.34	0.03
	30.0	317.51	317.52	0.01	294.01	294.04	0.03
	40.0	322.84	322.85	0.01	297.60	297.63	0.03



Table X. Theoretical Performance of  $N_2O_4/N_2H_4$  System  
 Chamber Pressure = 100 psia

Mixture Ratio	Area Ratio	Equilibrium Flow			Frozen Flow		
		All Species	9 Significant Species	$\Delta I_{sp}$	All Species	9 Significant Species	$\Delta I_{sp}$
0.5	10.0	288.09	288.09	0.00	287.46	287.46	0.00
	20.0	297.27	297.27	0.00	296.59	296.59	0.00
	30.0	301.54	301.53	0.01	300.83	300.83	0.00
	40.0	304.18	304.16	0.02	303.46	303.46	0.00
0.9	10.0	310.06	310.06	0.00	303.11	303.12	0.01
	20.0	321.77	321.77	0.00	314.00	314.00	0.00
	30.0	327.22	327.22	0.00	319.05	319.05	0.00
	40.0	330.58	330.58	0.00	322.16	322.17	0.01
1.1	10.0	314.68	314.68	0.00	302.44	302.44	0.00
	20.0	327.65	327.65	0.00	313.68	313.68	0.00
	30.0	333.76	333.76	0.00	318.91	318.92	0.01
	40.0	337.55	337.55	0.00	322.15	322.15	0.00
1.3	10.0	315.95	315.95	0.00	298.38	298.38	0.00
	20.0	330.24	330.24	0.00	309.65	309.65	0.00
	30.0	337.08	337.08	0.00	314.92	314.92	0.00
	40.0	341.35	341.35	0.00	318.18	318.18	0.00
2.0	10.0	290.92	290.93	0.01	276.98	276.99	0.01
	20.0	303.74	303.75	0.01	287.42	287.43	0.01
	30.0	309.84	309.84	0.00	292.31	292.32	0.01
	40.0	313.63	313.63	0.00	295.33	295.34	0.01

Table XI. Theoretical Performance of  $N_2O_4/N_2H_4$  System  
 Chamber Pressure = 1000 psia

Mixture Ratio	Area Ratio	Equilibrium Flow			Frozen Flow		
		All Species	9 Significant Species	$\Delta I_{3p}$	All Species	9 Significant Species	$I_{sp}$
0.5	10.0	288.11	288.11	0.00	287.90	287.90	0.00
	20.0	297.31	297.28	0.03	297.06	297.06	0.00
	30.0	301.60	301.54	0.06	301.31	301.31	0.00
	40.0	304.29	304.17	0.12	303.94	303.94	0.00
0.9	10.0	310.57	310.58	0.01	307.54	307.55	0.01
	20.0	322.16	322.16	0.00	318.78	318.78	0.00
	30.0	327.55	327.55	0.00	324.00	324.00	0.00
	40.0	330.87	330.87	0.00	327.22	327.23	0.01
1.1	10.0	315.96	315.96	0.00	309.48	309.49	0.01
	20.0	328.62	328.62	0.00	321.31	321.31	0.00
	30.0	334.59	334.59	0.00	326.84	326.85	0.01
	40.0	338.29	338.29	0.00	330.27	330.28	0.01
1.3	10.0	318.45	318.44	0.01	307.01	307.01	0.00
	20.0	332.18	332.19	0.01	319.01	319.02	0.01
	30.0	338.75	338.75	0.00	324.66	324.67	0.01
	40.0	342.85	342.85	0.00	328.17	328.18	0.01
2.0	10.0	292.43	292.44	0.01	283.06	283.08	0.02
	20.0	304.91	304.92	0.01	294.02	294.04	0.02
	30.0	310.84	310.84	0.00	299.16	299.18	0.02
	40.0	314.53	314.53	0.00	302.36	302.38	0.02

Table XII. Theoretical Performance of Compound A/N<sub>2</sub>H<sub>4</sub>  
 Chamber Pressure = 100 psia

Mixture Ratio	Area Ratio	Equilibrium Flow			Frozen Flow		
		All Species	11 Significant Species	$\Delta I_{sp}$	All Species	11 Significant Species	$\Delta I_{sp}$
1.0	10.0	312.43	312.43	0.00	304.68	304.69	0.01
	20.0	322.05	322.05	0.00	313.63	313.63	0.00
	30.0	326.41	326.41	0.00	317.70	317.70	0.00
	40.0	329.07	329.08	0.01	320.19	320.20	0.01
2.3	10.0	340.94	340.94	0.00	311.55	311.56	0.01
	20.0	355.27	355.27	0.00	320.42	320.43	0.01
	30.0	361.89	361.89	0.00	324.37	324.38	0.01
	40.0	365.92	365.92	0.00	326.76	326.77	0.01
2.5	10.0	341.63	341.63	0.00	312.42	312.43	0.01
	20.0	356.48	356.48	0.00	321.37	321.38	0.01
	30.0	363.42	363.42	0.00	325.36	325.37	0.01
	40.0	367.65	367.65	0.00	327.78	327.79	0.01
2.7	10.0	341.59	341.60	0.01	310.25	310.26	0.01
	20.0	356.86	356.86	0.00	319.02	319.04	0.02
	30.0	364.12	364.12	0.00	322.93	322.94	0.01
	40.0	368.60	368.60	0.00	325.29	325.30	0.01
5.0	10.0	263.30	263.30	0.00	238.27	238.27	0.00
	20.0	275.36	275.37	0.01	244.10	244.10	0.00
	30.0	281.01	281.01	0.00	246.72	246.72	0.00
	40.0	284.51	284.51	0.00	248.29	248.29	0.00

Table XIII Theoretical Performance of Compound A/N<sub>2</sub>H<sub>4</sub>  
Chamber Pressure, 1000 psia

Mixture Ratio	Area Ratio	Equilibrium Flow			Frozen Flow		
		All Species	11 Significant Species	$\Delta I_{sp}$	All Species	11 Significant Species	$\Delta I_{sp}$
1.0	10.0	312.84	312.84	0.00	309.46	309.47	0.01
	20.0	322.34	322.35	0.01	318.68	318.69	0.01
	30.0	326.66	326.66	0.00	322.87	322.88	0.01
	40.0	329.30	329.30	0.00	325.44	325.44	0.00
2.3	10.0	345.52	345.53	0.01	325.22	325.24	0.02
	20.0	358.71	358.71	0.00	335.06	335.08	0.02
	30.0	364.77	364.77	0.00	339.45	339.48	0.03
	40.0	368.46	368.46	0.00	342.11	342.14	0.03
2.5	10.0	346.79	346.79	0.00	324.51	324.53	0.03
	20.0	360.43	360.43	0.00	334.27	334.30	0.03
	30.0	366.73	366.74	0.01	338.63	338.66	0.03
	40.0	370.58	370.58	0.00	341.26	341.29	0.03
2.7	10.0	347.16	347.17	0.01	323.22	323.25	0.03
	20.0	361.31	361.31	0.00	332.87	332.91	0.04
	30.0	367.92	367.92	0.00	337.18	337.21	0.03
	40.0	371.96	371.97	0.01	339.78	339.81	0.03
5.0	10.0	269.48	269.49	0.01	247.86	247.86	0.00
	20.0	280.44	280.44	0.00	254.15	254.16	0.01
	30.0	285.69	285.70	0.01	257.00	257.00	0.00
	40.0	289.06	289.06	0.00	258.72	258.73	0.01

Table XIV. Theoretical Performance of  $N_2O_4/MMH$  System  
 Chamber Pressure = 100 psia

Mixture Ratio	Area Ratio	Equilibrium Flow			Frozen Flow		
		All Species	21 Significant Species	$\Delta I_{sp}$	All Species	21 Significant Species	$\Delta I_{sp}$
0.5	10.0	248.77	248.77	0.00	228.95	228.95	0.00
	20.0	261.37	261.37	0.00	235.58	235.57	0.01
	30.0	267.85	267.85	0.00	238.52	238.51	0.01
	40.0	272.11	272.11	0.00	240.24	240.24	0.00
1.5	10.0	304.66	304.66	0.00	295.75	295.76	0.01
	20.0	316.84	316.84	0.00	306.45	306.45	0.00
	30.0	322.68	322.68	0.00	311.42	311.43	0.01
	40.0	326.36	326.36	0.00	314.49	314.50	0.01
1.8	10.0	309.86	309.86	0.00	294.84	294.85	0.01
	20.0	323.42	323.42	0.00	305.92	305.92	0.00
	30.0	329.95	329.95	0.00	311.10	311.11	0.01
	40.0	334.07	334.07	0.00	314.31	314.31	0.00
2.1	10.0	310.76	310.76	0.00	290.57	290.57	0.00
	20.0	325.85	325.85	0.00	301.70	301.70	0.00
	30.0	333.18	333.18	0.00	306.92	306.93	0.01
	40.0	337.83	337.83	0.00	310.16	310.17	0.01
3.5	10.0	283.47	283.48	0.01	266.12	266.13	0.01
	20.0	297.25	297.25	0.00	276.42	276.43	0.01
	30.0	303.92	303.92	0.00	281.28	281.29	0.01
	40.0	308.13	308.14	0.01	284.30	284.31	0.01

Table XV. Theoretical Performance of  $N_2O_4/MMH$  System  
 Chamber Pressure = 1000 psia

Mixture Ratio	Area Ratio	Equilibrium Flow			Frozen Flow		
		All Species	21 Significant Species	$\Delta I_{sp}$	All Species	21 Significant Species	$\Delta I_{sp}$
0.5	10.0	256.22	256.23	0.01	237.69	237.69	0.00
	20.0	268.83	268.84	0.01	244.82	244.82	0.00
	30.0	275.28	275.30	0.02	248.06	248.06	0.00
	40.0	279.51	279.52	0.01	250.01	250.00	0.01
1.5	10.0	305.33	305.38	0.00	300.95	300.96	0.01
	20.0	317.40	317.40	0.00	312.06	312.07	0.01
	30.0	323.17	323.17	0.00	317.24	317.25	0.01
	40.0	326.81	326.81	0.00	320.44	320.45	0.01
1.8	10.0	311.71	311.71	0.00	302.90	302.91	0.01
	20.0	324.86	324.87	0.01	314.64	314.66	0.02
	30.0	331.21	331.21	0.00	320.17	320.19	0.02
	40.0	335.21	335.21	0.00	323.60	323.62	0.02
2.1	10.0	314.28	314.28	0.00	300.03	300.04	0.01
	20.0	328.62	328.64	0.00	311.95	311.97	0.02
	30.0	335.63	335.63	0.00	317.61	317.62	0.01
	40.0	340.06	340.06	0.00	321.13	321.14	0.01
3.5	10.0	286.10	286.11	0.01	273.39	273.41	0.02
	20.0	299.34	299.34	0.00	284.31	284.33	0.02
	30.0	305.75	305.75	0.00	289.50	289.52	0.02
	40.0	309.79	309.79	0.00	292.74	292.75	0.01

Table XVI. Theoretical Performance of OF<sub>2</sub>/MMH System  
 Chamber Pressure = 100 psia

Mixture Ratio	Area Ratio	Equilibrium Flow			Frozen Flow		
		All Species	27 Significant Species	$\Delta I_{sp}$	All Species	27 Significant Species	$\Delta I_{sp}$
0.5	10.0	294.08	294.08	0.00	289.10	289.11	0.01
	20.0	305.56	305.56	0.00	298.20	298.20	0.00
	30.0	311.46	311.46	0.00	302.44	302.44	0.00
	40.0	315.34	315.34	0.00	305.06	305.07	0.01
1.5	10.0	357.82	357.82	0.00	333.68	333.68	0.00
	20.0	371.75	371.75	0.00	343.74	343.75	0.01
	30.0	378.16	378.16	0.00	348.27	348.28	0.01
	40.0	382.07	382.07	0.00	351.03	351.03	0.00
1.8	10.0	364.08	364.08	0.00	333.69	333.70	0.01
	20.0	379.97	379.98	0.01	343.78	343.79	0.01
	30.0	387.43	387.43	0.00	348.32	348.32	0.00
	40.0	392.03	392.03	0.00	351.07	351.07	0.00
2.1	10.0	366.18	366.19	0.01	331.65	331.65	0.00
	20.0	383.86	383.86	0.00	341.63	341.64	0.01
	30.0	392.34	392.34	0.00	346.10	346.11	0.01
	40.0	397.62	397.62	0.00	348.82	348.83	0.01
3.5	10.0	355.12	355.12	0.00	316.22	316.23	0.01
	20.0	374.07	374.08	0.01	325.35	325.36	0.01
	30.0	383.77	383.77	0.00	329.43	329.43	0.01
	40.0	390.11	390.11	0.00	331.89	331.89	0.00

Table XVII. Theoretical Performance of OF<sub>2</sub>/MMH System  
 Chamber Pressure = 1000 psia

<u>Mixture Ratio</u>	<u>Area Ratio</u>	<u>Equilibrium Flow</u>			<u>Frozen Flow</u>		
		<u>All Species</u>	<u>27 Significant Species</u>	<u><math>\Delta I_{sp}</math></u>	<u>All Species</u>	<u>27 Significant Species</u>	<u><math>\Delta I_{sp}</math></u>
0.5	10.0	299.12	296.13	0.01	289.65	289.67	0.02
	20.0	308.24	308.24	0.00	298.81	298.82	0.01
	30.0	314.41	314.42	0.01	303.07	303.09	0.02
	40.0	318.46	318.46	0.00	305.72	305.73	0.01
1.5	10.0	360.88	360.88	0.00	345.85	345.88	0.03
	20.0	374.01	374.02	0.01	356.83	356.83	0.00
	30.0	380.06	380.06	0.00	361.76	361.76	0.00
	40.0	383.76	383.76	0.00	364.75	364.75	0.00
1.8	10.0	369.15	369.15	0.00	347.86	347.89	0.03
	20.0	383.83	383.84	0.01	359.00	359.03	0.03
	30.0	390.71	390.72	0.01	364.03	364.06	0.03
	40.0	394.95	394.96	0.01	367.08	367.11	0.03
2.1	10.0	373.37	373.38	0.01	346.71	346.74	0.03
	20.0	389.59	389.59	0.00	357.82	357.85	0.03
	30.0	397.28	397.28	0.00	362.84	362.87	0.03
	40.0	402.06	402.07	0.01	365.88	365.91	0.03
3.5	10.0	363.75	363.75	0.00	330.31	330.33	0.02
	20.0	382.30	382.31	0.01	340.46	340.47	0.01
	30.0	391.64	391.64	0.00	345.00	345.02	0.02
	40.0	397.65	397.65	0.00	347.74	347.76	0.02



Table XVIII. Theoretical Performance of ClOF<sub>3</sub>/MMH System  
 Chamber Pressure = 100 psia

Mixture Ratio	Area Ratio	Equilibrium Flow			Frozen Flow		
		All Species	32 Significant Species	$\Delta I_{sp}$	All Species	32 Significant Species	$\Delta I_{sp}$
0.5	10.0	254.45	254.45	0.00	243.34	243.34	0.00
	20.0	266.45	266.45	0.00	250.69	250.69	0.00
	30.0	272.62	272.62	0.00	254.07	254.07	0.00
	40.0	276.67	276.67	0.00	256.12	256.11	0.01
1.5	10.0	306.02	306.03	0.01	294.32	294.32	0.00
	20.0	317.54	317.55	0.01	304.06	304.07	0.01
	30.0	322.99	322.99	0.00	308.52	308.51	0.01
	40.0	326.41	326.41	0.00	311.26	311.25	0.01
1.8	10.0	311.90	311.91	0.01	293.77	293.78	0.01
	20.0	324.93	324.93	0.00	303.77	303.78	0.01
	30.0	331.10	331.11	0.01	308.35	308.36	0.01
	40.0	334.76	334.97	0.01	311.17	311.18	0.01
2.1	10.0	313.63	313.63	0.00	290.35	290.36	0.01
	20.0	328.24	328.24	0.00	300.35	300.36	0.01
	30.0	335.25	335.25	0.00	304.95	304.96	0.01
	40.0	339.65	339.65	0.00	307.77	307.78	0.01
3.5	10.0	294.11	294.13	0.02	268.73	268.76	0.03
	20.0	309.53	309.55	0.02	277.92	277.95	0.03
	30.0	317.20	317.22	0.02	282.15	282.17	0.02
	40.0	322.11	322.12	0.01	284.75	284.77	0.02

Table XIX. Theoretical Performance of ClO<sub>2</sub>/MMH System  
 Chamber Pressure = 1000 psia

Mixture Ratio	Area Ratio	Equilibrium Flow			Frozen Flow		
		All Species	32 Significant Species	$\Delta I_{sp}$	All Species	32 Significant Species	$\Delta I_{sp}$
0.5	10.0	259.96	259.97	0.01	246.91	246.91	0.00
	20.0	272.20	272.21	0.01	254.49	254.49	0.00
	30.0	278.45	278.46	0.01	257.99	257.99	0.00
	40.0	282.54	282.55	0.01	260.12	260.12	0.00
1.5	10.0	307.02	307.03	0.01	300.92	300.94	0.02
	20.0	318.29	318.31	0.02	311.15	311.17	0.02
	30.0	323.65	323.65	0.00	315.84	315.86	0.02
	40.0	327.01	327.00	0.01	318.72	318.74	0.02
1.8	10.0	314.18	314.19	0.01	303.09	303.12	0.03
	20.0	326.67	326.68	0.01	313.81	313.84	0.03
	30.0	332.61	332.61	0.00	318.76	318.79	0.03
	40.0	336.32	336.32	0.00	321.80	321.82	0.02
2.1	10.0	317.63	317.63	0.00	301.18	301.22	0.04
	20.0	331.37	331.38	0.01	312.05	312.09	0.04
	30.0	337.97	337.97	0.00	317.10	317.13	0.03
	40.0	342.10	342.10	0.00	320.19	320.23	0.04
3.5	10.0	299.59	299.63	0.04	278.90	278.98	0.08
	20.0	314.30	314.34	0.04	288.91	288.99	0.08
	30.0	321.52	321.55	0.03	293.56	293.63	0.07
	40.0	326.10	326.13	0.03	296.42	296.49	0.07

Table XX. Theoretical Performance of  $N_2H_4/B_2H_6$  System  
 Chamber Pressure = 100 psia

Mixture Ratio	Area Ratio	Equilibrium Flow			Frozen Flow		
		All Species	9 Significant Species	$\Delta I_{sp}$	All Species	9 Significant Species	$\Delta I_{sp}$
1.15	10.0	368.47	368.48	0.01	363.30	363.32	0.02
	20.0	385.60	385.60	0.00	379.82	379.84	0.02
	30.0	394.03	394.04	0.01	387.95	387.96	0.01
	40.0	399.43	399.43	0.00	393.14	393.15	0.01
1.25	10.0	365.63	365.63	0.00	362.80	362.85	0.05
	20.0	382.32	382.31	0.01	379.15	379.21	0.06
	30.0	390.50	390.50	0.00	387.18	387.24	0.06
	40.0	395.74	395.73	0.01	392.31	392.37	0.06
1.35	10.0	362.02	362.02	0.00	359.90	359.93	0.03
	20.0	378.26	378.26	0.00	375.90	375.94	0.04
	30.0	386.21	386.22	0.01	383.73	383.77	0.04
	40.0	391.28	391.28	0.00	388.72	388.76	0.04

Table XXI. Theoretical Performance of  $N_2H_4/B_2H_6$  System  
 Chamber Pressure = 1000 psia

<u>Mixture Ratio</u>	<u>Area Ratio</u>	<u>Equilibrium Flow</u>			<u>Frozen Flow</u>		
		<u>All Species</u>	<u>Significant Species</u>	$\Delta I_{sp}$	<u>All Species</u>	<u>Significant Species</u>	$\Delta I_{sp}$
1.15	10.0	368.81	368.84	0.03	366.59	366.71	0.12
	20.0	385.87	385.89	0.02	383.39	383.52	0.13
	30.0	394.28	394.29	0.01	391.67	391.80	0.13
	40.0	399.65	399.67	0.02	396.96	397.10	0.14
1.25	10.0	365.84	365.85	0.01	364.70	364.78	0.08
	20.0	382.48	382.48	0.00	381.21	381.29	0.08
	30.0	390.65	390.66	0.01	389.32	389.40	0.08
	40.0	395.87	395.87	0.00	394.50	394.58	0.08
1.35	10.0	362.18	362.18	0.00	361.38	361.42	0.04
	20.0	378.39	378.39	0.00	377.50	377.54	0.04
	30.0	386.33	386.33	0.00	385.39	385.44	0.05
	40.0	391.38	391.39	0.01	390.42	390.47	0.05

Table XXII. Theoretical Performance of  $\text{OF}_2/\text{B}_2\text{H}_6$  System  
 Chamber Pressure = 100 psia

Mixture Ratio	Area Ratio	Equilibrium Flow			Frozen Flow		
		All Species	18 Significant Species	$\Delta I_{sp}$	All Species	Significant Species	$\Delta I_{sp}$
2.4	10.0	380.05	380.16	0.11	351.00	351.13	0.13
	20.0	399.82	399.91	0.09	363.42	363.54	0.12
	30.0	409.90	409.98	0.08	369.21	369.32	0.11
	40.0	416.49	416.57	0.08	372.78	372.88	0.10
3.2	10.0	388.09	388.17	0.08	355.80	355.87	0.07
	20.0	408.71	408.78	0.07	368.17	368.24	0.07
	30.0	419.32	419.39	0.07	373.92	373.98	0.06
	40.0	426.31	426.37	0.06	377.46	377.52	0.06
4.0	10.0	390.36	390.37	0.01	355.15	355.12	0.03
	20.0	411.28	411.29	0.01	367.31	367.26	0.05
	30.0	422.03	422.04	0.01	372.94	372.89	0.05
	40.0	429.10	429.11	0.01	376.40	376.35	0.05

Table XXIII. Theoretical Performance of  $\text{OF}_2/\text{B}_2\text{H}_6$   
 Chamber Pressure = 1000 psia

Mixture Ratio	Area Ratio	Equilibrium Flow			Frozen Flow		
		All Species	18 Significant Species	$\Delta I_{sp}$	All Species	18 Significant Species	$\Delta I_{sp}$
2.4	10.0	387.64	387.87	0.23	364.44	364.76	0.32
	20.0	407.03	407.21	0.19	378.00	378.28	0.28
	30.0	416.96	417.14	0.18	384.38	384.65	0.27
	40.0	423.54	423.71	0.17	388.33	388.60	0.27
3.2	10.0	397.86	398.06	0.20	371.29	371.47	0.18
	20.0	418.35	418.52	0.17	384.94	385.10	0.16
	30.0	428.84	429.01	0.17	391.38	391.54	0.16
	40.0	435.75	435.90	0.15	395.38	395.52	0.14
4.0	10.0	400.50	400.57	0.07	371.13	371.10	0.03
	20.0	421.26	421.34	0.08	384.58	384.54	0.04
	30.0	431.81	431.89	0.07	390.93	390.87	0.06
	40.0	438.70	438.76	0.06	394.86	394.79	0.07

Table XXIV. Theoretical Performance of  $\text{OF}_2/\text{LiH}$  System  
 Chamber Pressure = 100 psia

Mixture Ratio	Area Ratio	Equilibrium Flow			Frozen Flow		
		All Species	16 Significant Species	$\Delta I_{sp}$	All Species	16 Significant Species	$\Delta I_{sp}$
2.5	10.0	346.73	346.76	0.03	322.10	322.19	0.09
	20.0	364.06	364.09	0.03	333.44	333.54	0.10
	30.0	372.91	373.93	0.02	338.72	338.82	0.10
	40.0	378.72	378.74	0.02	341.99	342.09	0.10
3.0	10.0	352.67	352.72	0.05	322.46	322.58	0.12
	20.0	371.27	371.32	0.05	333.66	333.79	0.13
	30.0	380.68	380.72	0.04	338.86	338.99	0.13
	40.0	386.79	386.83	0.04	342.07	342.19	0.12
3.5	10.0	351.84	351.89	0.05	320.09	320.23	0.14
	20.0	370.89	370.94	0.05	330.97	331.12	0.15
	30.0	380.66	380.70	0.04	336.00	336.15	0.15
	40.0	387.06	387.10	0.04	339.09	339.24	0.15

Table XXV. Theoretical Performance of  $OF_2/LiH$  System  
 Chamber Pressure = 1000 psia

Mixture Ratio	Area Ratio	Equilibrium Flow			Frozen Flow		
		All Species	16 Significant Species	$\Delta I_{sp}$	All Species	16 Significant Species	$\Delta I_{sp}$
2.5	10.0	354.00	354.04	0.04	335.21	335.35	0.14
	20.0	371.48	371.52	0.04	347.82	347.97	0.15
	30.0	380.41	380.45	0.04	353.78	353.93	0.15
	40.0	386.30	386.33	0.03	357.49	357.64	0.15
3.0	10.0	361.04	361.10	0.06	337.48	337.65	0.17
	20.0	379.22	379.74	0.04	350.01	350.18	0.17
	30.0	388.41	388.46	0.05	355.91	356.09	0.18
	40.0	394.42	394.47	0.05	359.58	359.76	0.18
3.5	10.0	361.02	361.09	0.07	335.49	335.67	0.18
	20.0	379.67	379.73	0.06	347.67	347.87	0.20
	30.0	389.14	389.20	0.06	353.40	353.60	0.20
	40.0	395.33	395.38	0.05	356.94	357.14	0.20



Table XXVI. Theoretical Performance of CTF/86% MMH+  
+14% N<sub>2</sub>H<sub>4</sub> System

Chamber Pressure = 100 psia

Mixture Ratio	Area Ratio	Equilibrium Flow			Frozen Flow		
		All Species	25 Significant Species	$\Delta I_{sp}$	All Species	25 Significant Species	$\Delta I_{sp}$
2.4	10.0	305.43	305.45	0.02	283.35	283.56	0.21
	20.0	318.46	318.48	0.02	292.71	292.92	0.21
	30.0	324.54	324.55	0.01	296.99	297.21	0.22
	40.0	328.28	328.29	0.01	299.62	299.84	0.22
2.8	10.0	306.97	307.01	0.04	281.68	282.04	0.36
	20.0	320.78	320.81	0.03	290.82	291.20	0.38
	30.0	327.28	327.31	0.03	295.00	295.39	0.39
	40.0	331.29	331.32	0.03	297.55	297.95	0.40
3.2	10.0	304.26	304.32	0.06	278.46	278.92	0.46
	20.0	317.30	317.34	0.04	287.35	287.84	0.49
	30.0	323.65	323.66	0.01	291.41	291.90	0.49
	40.0	327.72	327.68	0.04	293.87	294.39	0.49

Table XXVII. Theoretical Performance of CTF/86% MMH +  
+ 14% N<sub>2</sub>H<sub>4</sub> System

Chamber Pressure = 1000 psia

Mixture Ratio	Area Ratio	Equilibrium Flow			Frozen Flow		
		All Species	25 Significant Species	$\Delta I_{sp}$	All Species	25 Significant Species	$\Delta I_{sp}$
2.4	10.0	307.49	307.52	0.03	289.38	289.58	0.20
	20.0	320.02	320.04	0.02	299.28	299.48	0.20
	30.0	325.86	325.87	0.01	303.82	304.03	0.21
	40.0	329.45	329.47	0.02	306.61	306.83	0.22
2.8	10.0	309.92	309.96	0.04	287.92	288.23	0.31
	20.0	323.05	323.09	0.04	297.66	297.99	0.33
	30.0	329.21	329.24	0.03	302.13	302.46	0.33
	40.0	333.01	333.04	0.03	304.87	305.21	0.34
3.2	10.0	306.57	306.62	0.05	284.89	285.04	0.15
	20.0	319.54	319.49	0.05	294.41	294.58	0.17
	30.0	325.91	325.74	0.17	298.77	298.95	0.16
	40.0	329.96	329.67	0.29	301.44	301.62	0.18

Table XXVIII. Theoretical Performance of  
CTF/49% MMH+8% N<sub>2</sub>H<sub>4</sub>+43% Al

Chamber Pressure = 100 psia

Mixture Ratio	Area Ratio	Equilibrium Flow			Frozen Flow		
		All Species	35 Significant Species	$\Delta I_{sp}$	All Species	35 Significant Species	$\Delta I_{sp}$
2.5	10.0	295.19	295.52	0.33	267.94	268.09	0.15
	20.0	311.19	311.47	0.28	277.15	277.35	0.20
	30.0	319.41	319.68	0.27	281.41	281.64	0.23
	40.0	324.83	325.08	0.25	284.04	284.28	0.24
3.0	10.0	294.88	295.02	0.14	266.75	266.86	0.11
	20.0	310.96	311.08	0.12	275.73	275.87	0.14
	30.0	319.22	319.32	0.10	279.88	280.03	0.15
	40.0	324.64	324.74	0.10	282.42	282.59	0.17
3.5	10.0	292.48	292.56	0.08	264.69	264.83	0.14
	20.0	307.89	307.95	0.06	273.45	273.60	0.15
	30.0	315.45	315.51	0.06	277.49	277.65	0.16
	40.0	320.23	320.28	0.05	279.97	280.13	0.16

Table XXIX. Theoretical Performance of  
CTF/49% MMH+8% N<sub>2</sub>H<sub>4</sub>+43% Al

Chamber Pressure = 1000 psia

Mixture Ratio	Area Ratio	Equilibrium Flow			Frozen Flow		
		All Species	35 Significant Species	$\Delta I_{sp}$	All Species	35 Significant Species	$\Delta I_{sp}$
2.5	10.0	302.13	302.24	0.11	280.35	280.47	0.12
	20.0	318.15	318.24	0.09	290.64	290.79	0.15
	30.0	326.33	326.41	0.08	295.49	295.64	0.15
	40.0	331.68	331.76	0.08	298.49	298.66	0.17
3.0	10.0	301.82	301.92	0.10	279.06	279.19	0.13
	20.0	317.88	317.96	0.08	289.06	289.22	0.16
	30.0	326.04	326.11	0.07	293.75	293.92	0.17
	40.0	331.36	331.43	0.07	296.66	296.82	0.16
3.5	10.0	298.45	298.54	0.09	276.56	276.74	0.18
	20.0	312.93	313.00	0.07	286.27	286.45	0.18
	30.0	320.00	320.06	0.06	290.80	290.99	0.19
	40.0	324.53	324.57	0.04	293.60	293.79	0.19

Table XXX. Theoretical Performance of CTF/43%MMH +  
+7% N<sub>2</sub>H<sub>4</sub>+50% B

Chamber Pressure = 100 psia

Mixture Ratio	Area Ratio	Equilibrium Flow			Frozen Flow		
		All Species	39 Significant Species	$\Delta I_{sp}$	All Species	39 Significant Species	$\Delta I_{sp}$
4.0	10.0	288.95	289.09	0.14	263.45	263.37	0.08
	20.0	305.12	305.24	0.12	273.00	272.95	0.05
	30.0	313.51	313.63	0.12	277.49	277.45	0.04
	40.0	319.07	319.18	0.11	280.28	280.24	0.04
5.0	10.0	291.82	291.89	0.07	264.37	264.35	0.02
	20.0	308.30	308.36	0.06	273.76	273.74	0.02
	30.0	316.82	316.89	0.07	278.15	278.14	0.01
	40.0	322.46	322.52	0.06	280.88	280.87	0.01
6.0	10.0	291.96	291.99	0.03	263.00	263.06	0.06
	20.0	308.50	308.55	0.05	272.17	272.23	0.05
	30.0	317.09	317.13	0.04	276.46	276.52	0.06
	40.0	322.75	322.79	0.04	279.11	279.17	0.06

Table XXXI. Theoretical Performance of CTF/43% MMH+  
+7% N<sub>2</sub>H<sub>4</sub>+50% B

Chamber Pressure = 1000 psia

Mixture Ratio	Area Ratio	Equilibrium Flow			Frozen Flow		
		All Species	39 Significant Species	$\Delta I_{sp}$	All Species	39 Significant Species	$\Delta I_{sp}$
4.0	10.0	296.55	296.64	0.09	275.73	275.73	0.00
	20.0	312.87	312.95	0.08	286.35	286.37	0.02
	30.0	321.32	321.39	0.07	291.44	291.46	0.02
	40.0	326.91	326.98	0.07	294.62	294.65	0.03
5.0	10.0	299.71	299.77	0.06	276.87	276.94	0.07
	20.0	316.29	316.35	0.06	287.27	287.34	0.07
	30.0	324.86	324.92	0.06	292.23	292.30	0.07
	40.0	330.52	330.58	0.04	295.32	295.40	0.08
6.0	10.0	300.03	300.10	0.07	275.53	275.65	0.12
	20.0	316.29	316.37	0.08	285.64	285.78	0.14
	30.0	324.64	324.71	0.07	290.44	290.58	0.14
	40.0	330.07	330.13	0.06	293.44	293.57	0.13

Table XXXII. Theoretical Performance of CTF/45% MMH+  
+7% N<sub>2</sub>H<sub>4</sub>+50% Be

Chamber Pressure = 100 psia

Mixture Ratio	Area Ratio	Equilibrium Flow			Frozen Flow		
		All Species	31 Significant Species	$\Delta I_{sp}$	All Species	Significant Species	$\Delta I_{sp}$
3.5	10.0	309.82	309.98	0.16	283.86	283.77	0.09
	20.0	326.98	327.13	0.15	294.12	294.04	0.08
	30.0	335.88	336.02	0.14	298.95	298.88	0.07
	40.0	341.78	341.91	0.13	301.95	391.89	0.06
4.5	10.0	310.36	310.43	0.07	282.28	282.07	0.21
	20.0	327.39	327.47	0.08	292.16	291.94	0.22
	30.0	336.15	336.22	0.07	296.77	296.56	0.21
	40.0	341.92	341.99	0.07	299.64	299.42	0.22
5.5	10.0	306.16	306.22	0.06	277.60	277.57	0.03
	20.0	321.84	321.79	0.05	287.04	287.01	0.03
	30.0	329.47	329.52	0.05	291.42	291.41	0.01
	40.0	334.30	334.34	0.04	294.14	294.12	0.02

Table XXXIII. Theoretical Performance of CTF/45% MMH +  
+7% N<sub>2</sub>H<sub>4</sub>+50% Be

Chamber Pressure = 1000 psia

<u>Mixture Ratio</u>	<u>Area Ratio</u>	<u>Equilibrium Flow</u>			<u>Frozen Flow</u>		
		<u>All Species</u>	<u>31 Significant Species</u>	<u><math>\Delta I_{sp}</math></u>	<u>All Species</u>	<u>31 Significant Species</u>	<u><math>\Delta I_{sp}</math></u>
3.5	10.0	318.41	318.50	0.09	297.23	297.24	0.01
	20.0	335.57	335.66	0.09	308.51	308.54	0.03
	30.0	344.44	344.53	0.09	313.91	313.95	0.04
	40.0	350.30	350.38	0.08	317.29	317.33	0.04
4.5	10.0	318.50	318.56	0.06	295.31	295.25	0.06
	20.0	335.44	335.50	0.06	306.15	306.10	0.05
	30.0	344.10	344.16	0.06	311.29	311.24	0.05
	40.0	349.76	349.81	0.05	314.50	314.45	0.05
5.5	10.0	312.58	312.64	0.06	290.01	290.07	0.06
	20.0	327.15	327.21	0.06	300.32	300.39	0.07
	30.0	334.27	334.31	0.04	305.18	305.24	0.06
	40.0	338.84	338.86	0.02	308.19	308.26	0.07



Table XXXIV. Theoretical Performance of AP/PBAA-Al System

Chamber Pressure (psia)	Area Ratio	Equilibrium Flow			Frozen Flow		
		All Species	34 Significant Species	$\Delta I_{sp}$	All Species	34 Significant Species	$\Delta I_{sp}$
100	10.0	283.70	283.71	0.01	270.33	270.35	0.02
	20.0	299.29	299.29	0.00	282.14	282.16	0.02
	30.0	307.05	307.05	0.00	287.89	287.91	0.02
	40.0	312.03	312.04	0.01	291.52	291.55	0.03
1000	10.0	286.52	286.54	0.02	277.34	277.38	0.04
	20.0	301.70	301.70	0.00	289.74	289.78	0.04
	30.0	309.22	309.22	0.00	295.82	295.87	0.05
	40.0	314.04	314.04	0.00	299.70	299.74	0.04

Table XXXV. Theoretical Performance of AP/PBAA-Be System

Chamber Pressure (psia)	Area Ratio	Equilibrium Flow			Frozen Flow		
		All Species	34 Significant Species	$\Delta I_{sp}$	All Species	34 Significant Species	$\Delta I_{sp}$
100	10.0	305.71	305.74	0.03	289.32	289.45	0.13
	20.0	324.00	324.03	0.03	303.10	303.25	0.15
	30.0	333.39	333.41	0.03	309.93	310.09	0.16
	40.0	339.56	339.57	0.01	314.32	314.48	0.16
1000	10.0	308.84	308.87	0.03	296.54	296.68	0.14
	20.0	327.15	327.18	0.03	311.01	311.16	0.15
	30.0	336.46	336.48	0.02	318.25	318.40	0.15
	40.0	342.53	342.55	0.02	322.91	323.07	0.16

Table XXXVI. Theoretical Performance of AP/DB-A1

Chamber Pressure (psia)	Area Ratio	Equilibrium Flow			Frozen Flow		
		All Species	34 Significant Species	$\Delta I_{up}$	All Species	34 Significant Species	$\Delta I_{sp}$
100	10.0	284.61	284.62	0.01	272.41	272.47	0.06
	20.0	300.70	300.73	0.03	284.76	284.83	0.07
	30.0	309.26	309.24	0.02	290.86	290.93	0.07
	40.0	314.82	314.78	0.04	294.76	294.83	0.07
1000	10.0	288.46	288.47	0.01	280.52	280.64	0.12
	20.0	304.20	304.20	0.00	293.53	293.67	0.14
	30.0	312.50	312.51	0.01	300.01	300.15	0.14
	40.0	317.87	317.89	0.02	304.18	304.32	0.14

Table XXXVII. Theoretical Performance of AP/DB-Be System

Chamber Pressure (psia)	Area Ratio	Equilibrium Flow			Frozen Flow		
		All Species	34 Significant Species	$\Delta I_{op}$	All Species	34 Significant Species	$\Delta I_{op}$
100	10.0	303.92	304.00	0.08	289.89	290.18	0.29
	20.0	322.16	322.23	0.07	303.67	304.00	0.33
	30.0	331.52	331.58	0.06	310.52	310.88	0.36
	40.0	337.66	337.72	0.06	314.92	315.30	0.38
1000	10.0	307.68	307.72	0.04	298.31	298.48	0.17
	20.0	325.93	325.97	0.04	312.87	313.06	0.19
	30.0	335.20	335.23	0.03	320.18	320.38	0.20
	40.0	341.24	341.27	0.03	324.90	325.10	0.20

APPENDIX B

Table 1. Chemical Reactions of Importance in Nonmetallized Propellant Systems Containing Carbon, Hydrogen, Oxygen, Nitrogen, Fluorine and Chlorine Having Gaseous Combustion Products

<u>Chemical Reaction</u>	<u>Chemical Reaction</u>
$\text{CO}_2 + \text{M} \rightleftharpoons \text{CO} + \text{O} + \text{M}$	$\text{HCl} + \text{HCl} \rightleftharpoons \text{H}_2 + \text{Cl}_2$
$\text{H}_2\text{O} + \text{M} \rightleftharpoons \text{OH} + \text{H} + \text{M}$	$\text{HCl} + \text{O} \rightleftharpoons \text{OH} + \text{Cl}$
$\text{CO} + \text{M} \rightleftharpoons \text{C} + \text{O} + \text{M}$	$\text{HF} + \text{Cl} \rightleftharpoons \text{HCl} + \text{F}$
$\text{Cl}_2 + \text{M} \rightleftharpoons 2\text{Cl} + \text{M}$	$\text{HF} + \text{F} \rightleftharpoons \text{H} + \text{F}_2$
$\text{F}_2 + \text{M} \rightleftharpoons 2\text{F} + \text{M}$	$\text{HF} + \text{H} \rightleftharpoons \text{H}_2 + \text{F}$
$\text{HCl} + \text{M} \rightleftharpoons \text{H} + \text{Cl} + \text{M}$	$\text{HF} + \text{HF} \rightleftharpoons \text{H}_2 + \text{F}_2$
$\text{HF} + \text{M} \rightleftharpoons \text{H} + \text{F} + \text{M}$	$\text{HF} + \text{O} \rightleftharpoons \text{OH} + \text{F}$
$\text{H}_2 + \text{M} \rightleftharpoons 2\text{H} + \text{M}$	$\text{HF} + \text{OH} \rightleftharpoons \text{H}_2\text{O} + \text{F}$
$\text{N}_2 + \text{M} \rightleftharpoons 2\text{N} + \text{M}$	$\text{H}_2 + \text{Cl} \rightleftharpoons \text{HCl} + \text{H}$
$\text{NO} + \text{M} \rightleftharpoons \text{N} + \text{O} + \text{M}$	$\text{H}_2 + \text{O} \rightleftharpoons \text{OH} + \text{H}$
$\text{OH} + \text{M} \rightleftharpoons \text{O} + \text{H} + \text{M}$	$\text{H}_2 + \text{O}_2 \rightleftharpoons 2\text{OH}$
$\text{O}_2 + \text{M} \rightleftharpoons 2\text{O} + \text{M}$	$\text{N}_2 + \text{O} \rightleftharpoons \text{NO} + \text{N}$
$\text{ClF} + \text{M} \rightleftharpoons \text{Cl} + \text{F} + \text{M}$	$\text{N}_2 + \text{O}_2 \rightleftharpoons 2\text{NO}$
$\text{CO}_2 + \text{H} \rightleftharpoons \text{CO} + \text{OH}$	$\text{NO} + \text{H} \rightleftharpoons \text{N} + \text{OH}$
$\text{CO}_2 + \text{O} \rightleftharpoons \text{CO} + \text{O}_2$	$\text{NO} + \text{O} \rightleftharpoons \text{N} + \text{O}_2$
$\text{H}_2\text{O} + \text{Cl} \rightleftharpoons \text{OH} + \text{HCl}$	$\text{O}_2 + \text{H} \rightleftharpoons \text{OH} + \text{O}$
$\text{H}_2\text{O} + \text{H} \rightleftharpoons \text{OH} + \text{H}_2$	$\text{Cl} + \text{ClF} \rightleftharpoons \text{Cl}_2 + \text{F}$
$\text{H}_2\text{O} + \text{O} \rightleftharpoons 2\text{OH}$	$\text{F} + \text{ClF} \rightleftharpoons \text{Cl} + \text{F}_2$
$\text{CO} + \text{CO} \rightleftharpoons \text{CO}_2 + \text{C}$	$\text{HF} + \text{Cl} \rightleftharpoons \text{ClF} + \text{H}$
$\text{CO} + \text{H} \rightleftharpoons \text{C} + \text{OH}$	$\text{HCl} + \text{F} \rightleftharpoons \text{ClF} + \text{H}$
$\text{CO} + \text{N} \rightleftharpoons \text{C} + \text{NO}$	$\text{HCl} + \text{HF} \rightleftharpoons \text{ClF} + \text{H}_2$
$\text{CO} + \text{NO} \rightleftharpoons \text{CO}_2 + \text{N}$	$\text{HF} + \text{ClF} \rightleftharpoons \text{F}_2 + \text{HCl}$
$\text{CO} + \text{O} \rightleftharpoons \text{C} + \text{O}_2$	$\text{HF} + \text{Cl}_2 \rightleftharpoons \text{ClF} + \text{HCl}$
$\text{HCl} + \text{Cl} \rightleftharpoons \text{H} + \text{Cl}_2$	$\text{ClF} + \text{ClF} \rightleftharpoons \text{F}_2 + \text{Cl}_2$

Table II. Additional Chemical Reactions of Importance in Propellant Systems Containing Condensed Carbon As a Combustion Product

<u>Chemical Reaction</u>	<u>Chemical Reaction</u>
$C_2 + M = C + C + M$	$CO + F = CF + O$
$CH + M = C + H + M$	$CO + H = CH + O$
$CH_2 + M = CH + H + M$	$CO + H_2 = CH + OH$
$CH_3 + M = CH_2 + H + M$	$CO + HF = CF + OH$
$CH_4 + M = CH_3 + H + M$	$CO + N = CN + O$
$C_2H_2 + M = CH + CH + M$	$CO + N_2 = CN + NO$
$CN + M = C + N + M$	$CO + OH = CH + O_2$
$HCN + M = CN + H + M$	$C + CO = C_2 + O$
$CNCl + M = CN + Cl + M$	$CO + CO = C_2 + O_2$
$CNF + M = F + CN + M$	$F + CNCl = CN + ClF$
$CF + M = C + F + M$	$HCl + CNF = HCN + ClF$
$C_2F_2 + M = CF + CF + M$	$HF + CNCl = HCN + ClF$
$HCN + M = CH + N + M$	$ClF + CNF = CNCl + F_2$
$CNF + M = CF + N + M$	$Cl_2 + CNF = CNCl + ClF$
$F + CF = F_2 + C$	$C + HCN = CH + CN$
$C + H_2 = CH + H$	$C + CNF = CF + CN$
$C + H_2O = CH + OH$	$C + CH_3 = CH + CH_2$
$C + HF = CH + F$	$C + CH_2 = CH + CH$
$C + HF = CF + H$	$CH + HCN = CN + CH_2$
$C + HCl = CH + Cl$	$HCN + CF = CNF + CH$
$C + N_2 = CN + N$	$CH_4 + C = CH_3 + CH$
$O + CN = NO + C$	$HCN + CH_2 = CH_3 + CN$
$C + OH = CH + O$	$HCN + CH_3 = CH_4 + CN$
$Cl + CF = ClF + C$	$CH_3 + CH = CH_2 + CH_2$

Table II. (continued)

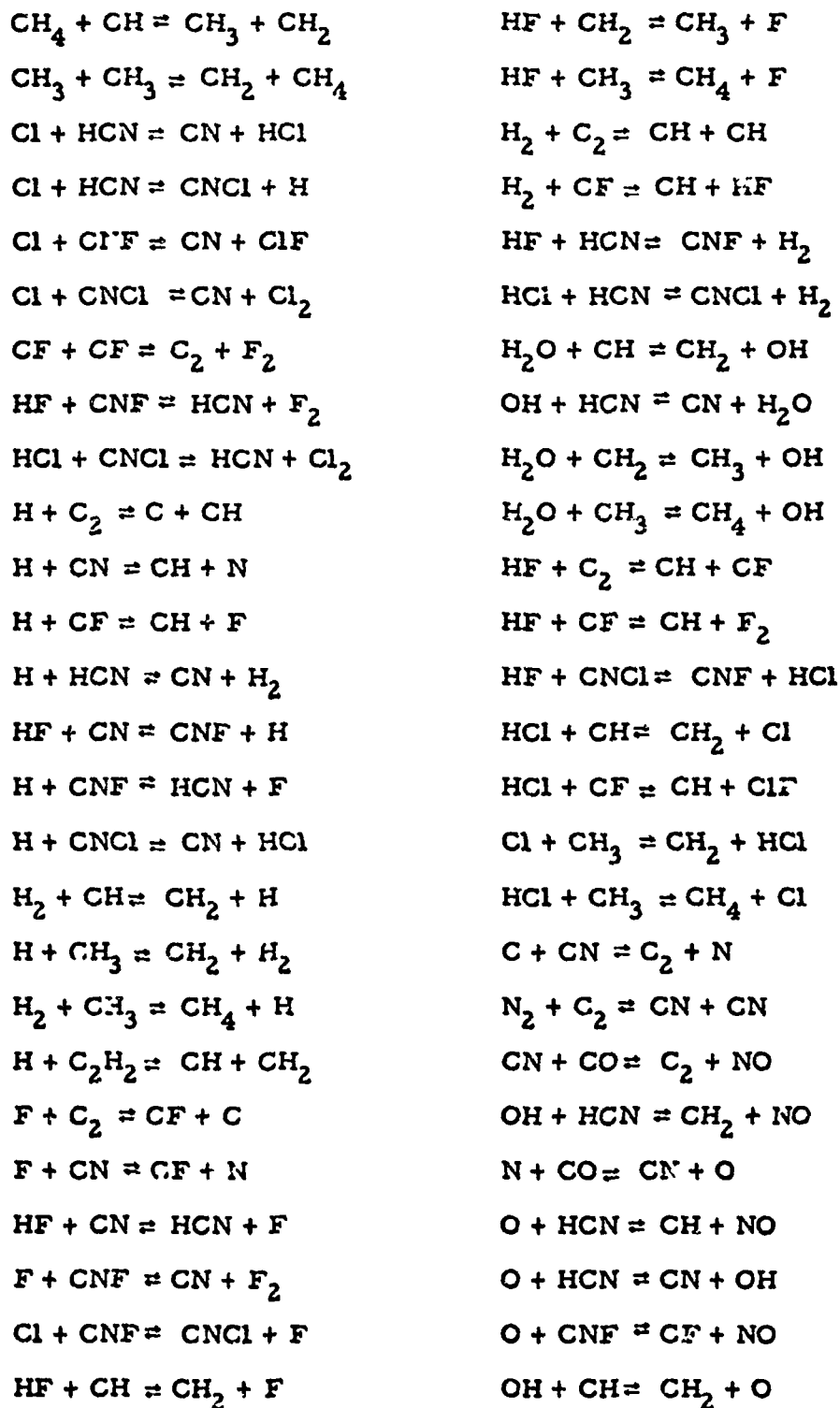




Table II. (continued)

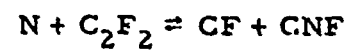
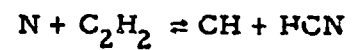
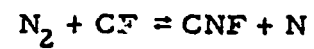
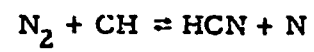
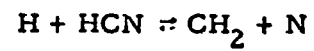
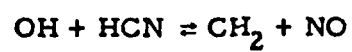
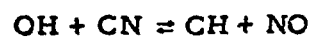
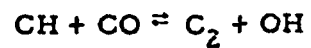
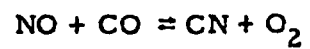
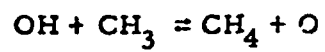
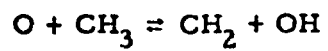


Table III. Additional Chemical Reactions of Importance in Aluminum Containing Propellant Systems

<u>Chemical Reaction</u>	<u>Chemical Reaction</u>
$AlO + M = Al + O + M$	$Al + AlOCl = AlO + AlCl$
$Al_2O + M = Al + AlO + M$	$Al + AlOF = Al_2O + F$
$AlCl + M = Al + Cl + M$	$OH + AlF = HF + AlO$
$AlCl_2 + M = AlCl + Cl + M$	$O + AlF = F + AlO$
$AlCl_3 + M = AlCl_2 + Cl + M$	$AlO + H = Al + OH$
$AlF + M = Al + F + M$	$AlO + AlF = Al_2O + F$
$AlF_2 + M = AlF + F + M$	$AlOF + Al = AlF + AlO$
$AlF_3 + M = AlF_2 + F + M$	$Al_2O + Cl = AlO + AlCl$
$AlOCl + M = AlO + Cl + M$	$Al_2O + O = AlO + AlO$
$AlOF + M = AlO + F + M$	$AlCl + CO = AlOCl + C$
$AlClF + M = AlF + Cl + M$	$AlCl + HCl = AlCl_2 + H$
$AlCl_2F + M = AlCl_2 + F + M$	$AlCl + NO = AlOCl + N$
$AlClF_2 + M = AlF_2 + Cl + M$	$AlCl + OH = AlO + HCl$
$AlOCl + M = AlCl + O + M$	$AlCl + Cl = Al + Cl_2$
$AlOF + M = AlF + O + M$	$AlCl + H = Al + HCl$
$AlClF + M = AlCl + F + M$	$AlCl + O = AlO + Cl$
$AlCl_2F + M = AlClF + Cl + M$	$AlCl + AlCl = Al + AlCl_2$
$AlClF_2 + M = AlClF + F + M$	$AlCl + AlOCl = Al_2O + Cl_2$
$Al + CO_2 = AlO + CO$	$AlCl + AlOCl = AlO + AlCl_2$
$Al + CO = AlO + C$	$AlCl + AlOF = AlF + AlOCl$
$Al + NO = AlO + N$	$AlCl_2 + Cl = AlCl + Cl_2$
$Al + O_2 = AlO + O$	$AlOCl + CO = AlCl + CO_2$
$Al + AlOCl = Al_2O + Cl$	$AlOCl + HCl = AlCl_2 + OH$

Table III. (continued)

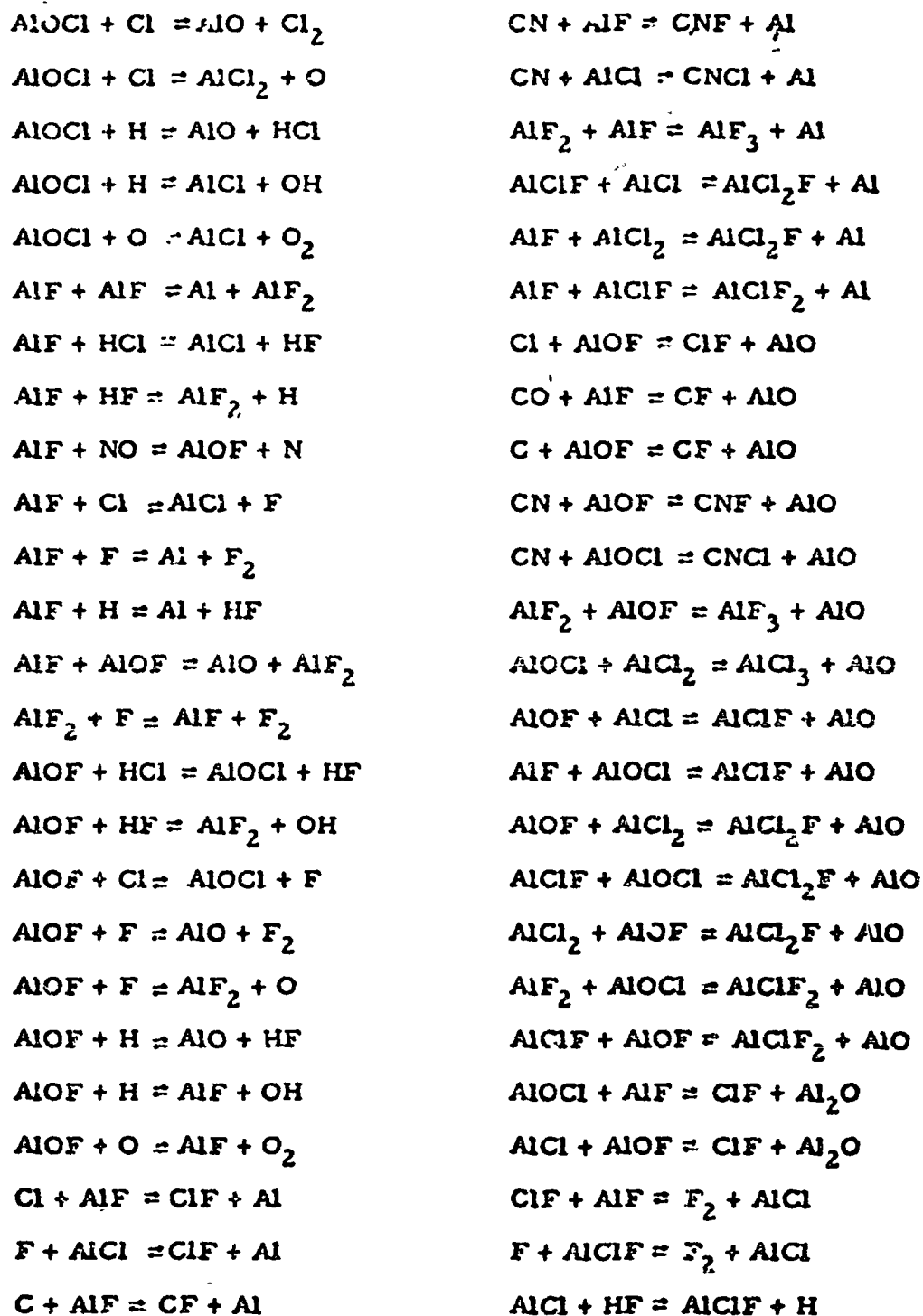


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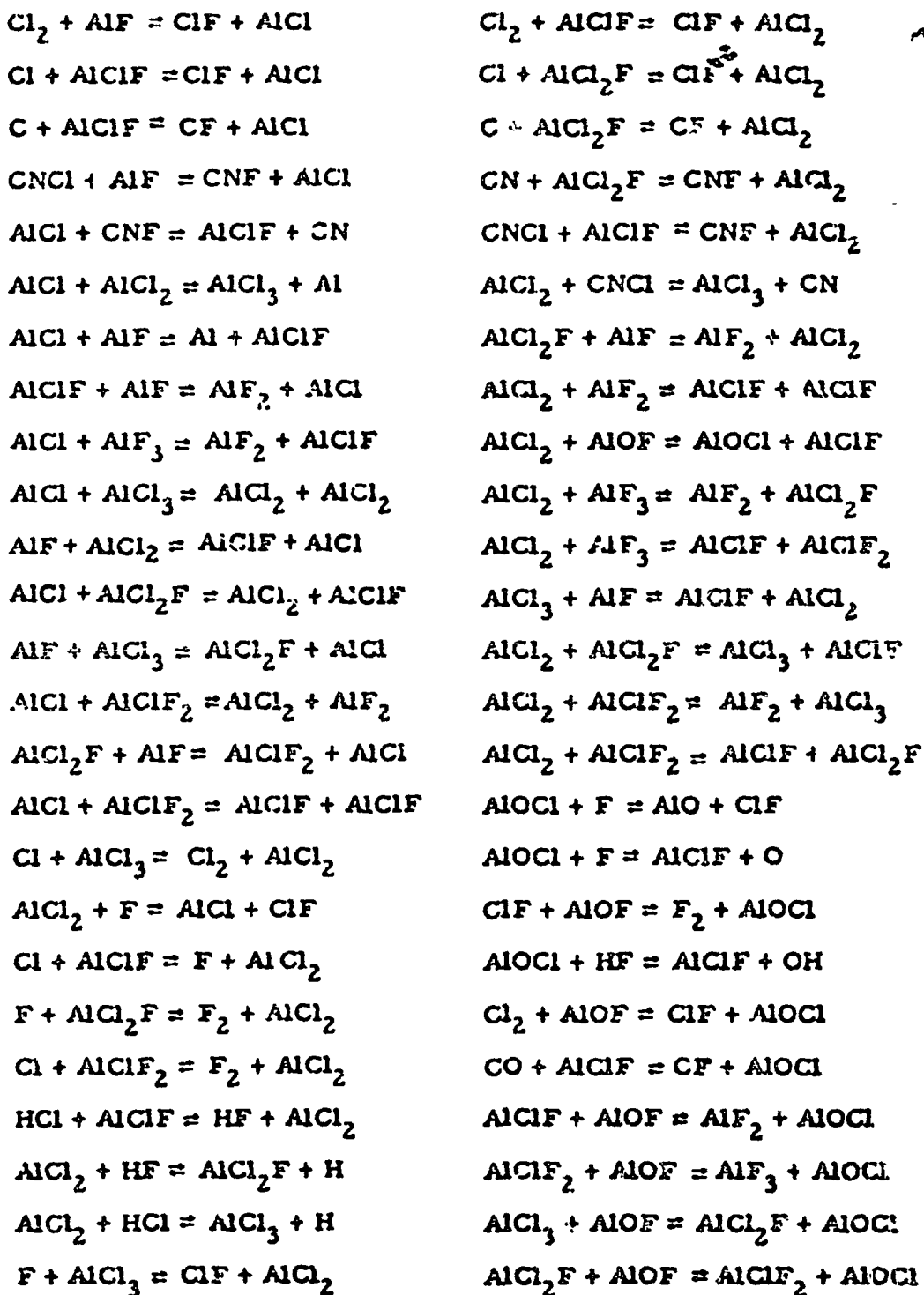


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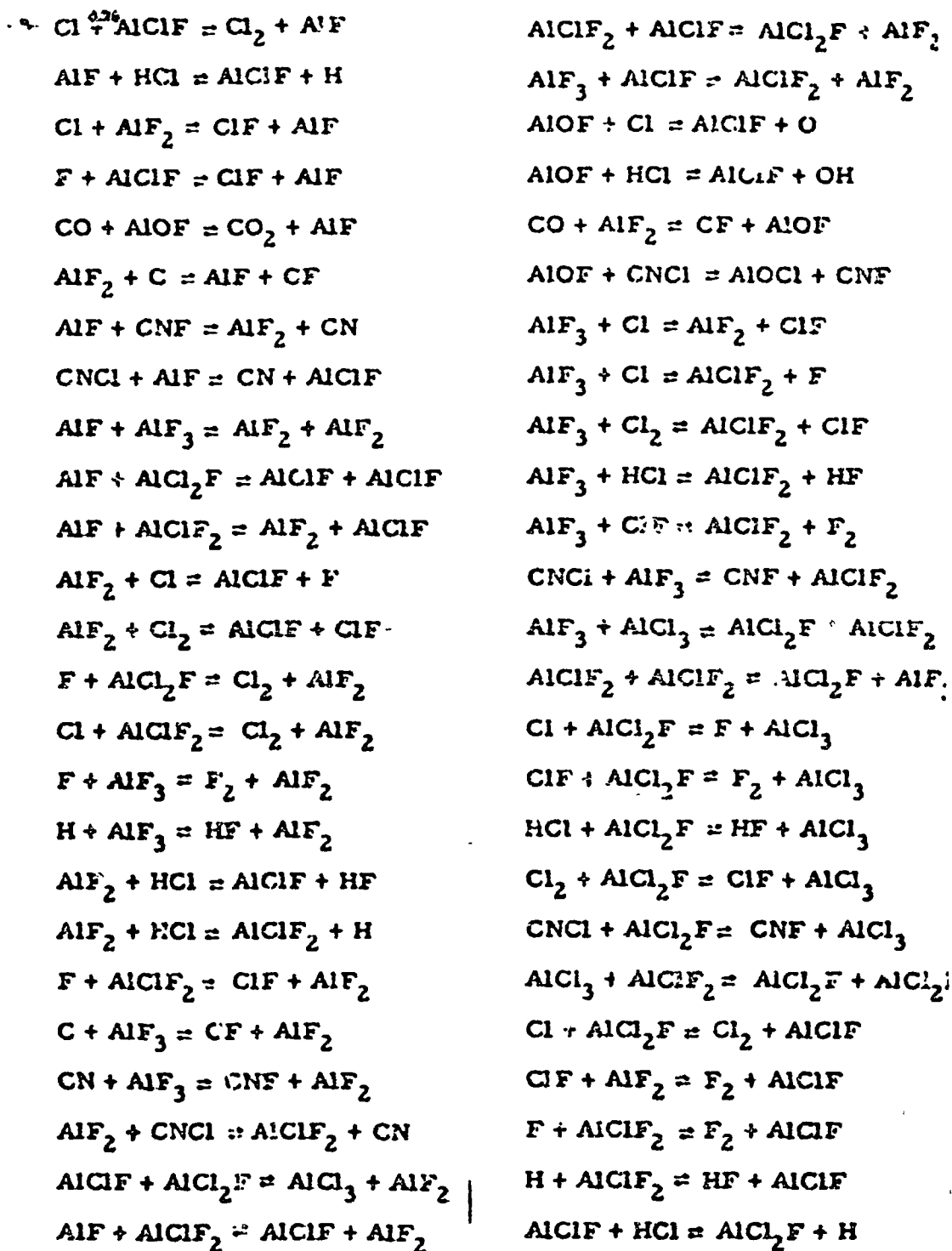


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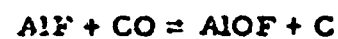
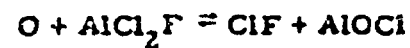
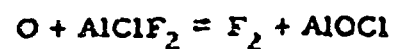
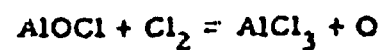
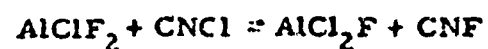
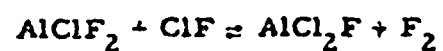
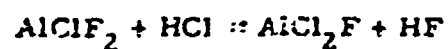
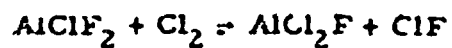
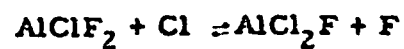
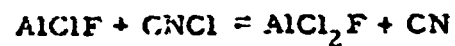
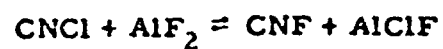
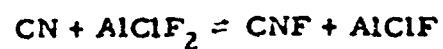
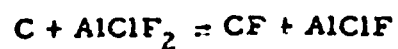
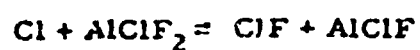
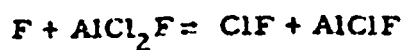
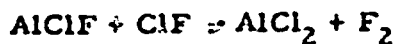


Table IV. Additional Chemical Reactions of Importance in Beryllium Containing Propellant Systems

<u>Chemical Reactions</u>	<u>Chemical Reactions</u>
$\text{BeOH} + \text{M} \rightleftharpoons \text{Be} + \text{OH} + \text{M}$	$\text{Be}_2\text{O} + \text{HF} \rightleftharpoons \text{BeF} + \text{BeOH}$
$\text{BeOH}_2 + \text{M} \rightleftharpoons \text{BeOH} + \text{OH} + \text{M}$	$\text{Be}_2\text{O} + \text{OH} \rightleftharpoons \text{BeO} + \text{BeOH}$
$\text{BeO} + \text{M} \rightleftharpoons \text{Be} + \text{O} + \text{M}$	$\text{Be}_2\text{O} + \text{Cl} \rightleftharpoons \text{BeO} + \text{BeCl}$
$\text{Be}_2\text{O} + \text{M} \rightleftharpoons \text{Be} + \text{BeO} + \text{M}$	$\text{Be}_2\text{O} + \text{H} \rightleftharpoons \text{Be} + \text{BeOH}$
$\text{BeCl} + \text{M} \rightleftharpoons \text{Be} + \text{Cl} + \text{M}$	$\text{Be}_2\text{O} + \text{O} \rightleftharpoons \text{BeO} + \text{BeO}$
$\text{BeCl}_2 + \text{M} \rightleftharpoons \text{BeCl} + \text{Cl} + \text{M}$	$\text{BeOH}_2 + \text{Be} \rightleftharpoons \text{BeOH} + \text{BeOH}$
$\text{BeF} + \text{M} \rightleftharpoons \text{Be} + \text{F} + \text{M}$	$\text{BeOH} + \text{Cl} \rightleftharpoons \text{BeO} + \text{HCl}$
$\text{BeF}_2 + \text{M} \rightleftharpoons \text{BeF} + \text{F} + \text{M}$	$\text{BeOH} + \text{Cl} \rightleftharpoons \text{BeCl} + \text{OH}$
$\text{BeOH} + \text{M} \rightleftharpoons \text{BeO} + \text{H} + \text{M}$	$\text{H}_2\text{O} + \text{Be} \rightleftharpoons \text{H} + \text{BeOH}$
$\text{BeClF} + \text{M} \rightleftharpoons \text{BeCl} + \text{F} + \text{M}$	$\text{BeOH} + \text{H} \rightleftharpoons \text{BeO} + \text{H}_2$
$\text{BeClF} + \text{M} \rightleftharpoons \text{BeF} + \text{Cl} + \text{M}$	$\text{BeOH} + \text{O} \rightleftharpoons \text{BeO} + \text{OH}$
$\text{Be} + \text{BeF}_2 \rightleftharpoons \text{BeF} + \text{BeF}$	$\text{Be} + \text{BeCl}_2 \rightleftharpoons \text{BeCl} + \text{BeCl}$
$\text{BeO} + \text{H}_2\text{O} \rightleftharpoons \text{BeOH} + \text{OH}$	$\text{BeCl} + \frac{1}{2}\text{O}_2 \rightleftharpoons \text{BeOH} + \text{HCl}$
$\text{CO}_2 + \text{Be} \rightleftharpoons \text{CO} + \text{BeO}$	$\text{H} + \text{BeCl}_2 \rightleftharpoons \text{HCl} + \text{BeCl}$
$\text{BeO} + \text{HCl} \rightleftharpoons \text{BeCl} + \text{OH}$	$\text{BeCl} + \text{Cl} \rightleftharpoons \text{Be} + \text{Cl}_2$
$\text{BeO} + \text{HF} \rightleftharpoons \text{BeOH} + \text{F}$	$\text{BeCl} + \text{H} \rightleftharpoons \text{Be} + \text{HCl}$
$\text{CO} + \text{Be} \rightleftharpoons \text{C} + \text{BeO}$	$\text{BeF} + \text{H}_2\text{O} \rightleftharpoons \text{BeOH} + \text{HF}$
$\text{BeO} + \text{Cl} \rightleftharpoons \text{BeCl} + \text{O}$	$\text{BeF} + \text{HCl} \rightleftharpoons \text{BeCl} + \text{HF}$
$\text{BeO} + \text{H} \rightleftharpoons \text{Be} + \text{OH}$	$\text{BeF} + \text{OH} \rightleftharpoons \text{BeO} + \text{HF}$
$\text{NO} + \text{Be} \rightleftharpoons \text{N} + \text{BeO}$	$\text{BeF} + \text{OH} \rightleftharpoons \text{BeOH} + \text{F}$
$\text{O}_2 + \text{Be} \rightleftharpoons \text{O} + \text{BeO}$	$\text{BeF} + \text{Cl} \rightleftharpoons \text{BeCl} + \text{F}$
$\text{BeO} + \text{BeF} \rightleftharpoons \text{Be}_2\text{O} + \text{F}$	$\text{BeF} + \text{F} \rightleftharpoons \text{Be} + \text{F}_2$
$\text{Be}_2\text{O} + \text{H}_2\text{O} \rightleftharpoons \text{BeOH} + \text{BeOH}$	$\text{BeF} + \text{H} \rightleftharpoons \text{Be} + \text{HF}$
$\text{Be}_2\text{O} + \text{HCl} \rightleftharpoons \text{BeCl} + \text{BeOH}$	$\text{BeF} + \text{O} \rightleftharpoons \text{BeO} + \text{F}$

Table IV. (continued)

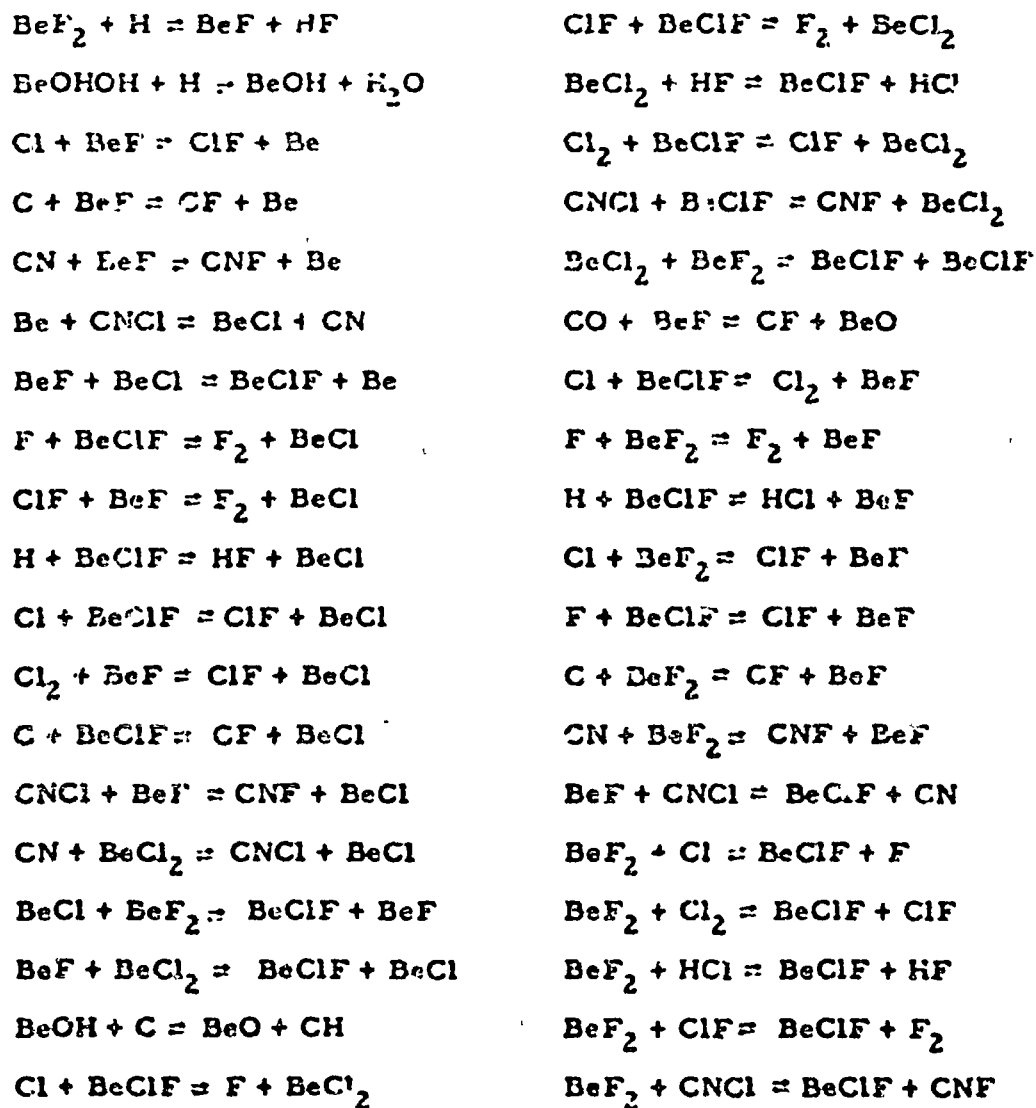




Table V. Additional Chemical Reactions of Importance in Boron Containing Propellant Systems

<u>Chemical Reaction</u>	<u>Chemical Reaction</u>
$BN + M = B + N + M$	$BO + BO = B + BO_2$
$BO + M = B + O + M$	$CO + BO_2 = CO_2 + BO$
$BO_2 + M = BO + O + M$	$BO + CO = B + CO_2$
$BCl + M = B + Cl + M$	$BO + CO = BO_2 + C$
$BCl_2 + M = BCl + Cl + M$	$BO + HCl = BCl + OH$
$BCl_3 + M = BCl_2 + Cl + M$	$BO + HF = BF + OH$
$BF + M = B + F + M$	$BO + NO = BN + O_2$
$BF_2 + M = BF + F + M$	$BO + NO = BO_2 + N$
$BF_3 + M = BF_2 + F + M$	$CO + B = C + BO$
$BOCl + M = BCl + O + M$	$BO + Cl = BCl + O$
$BOF + M = BO + F + M$	$BO + F = BF + O$
$BClF + M = BF + Cl + M$	$BO + H = B + OH$
$BCl_2F + M = BCl_2 + F + M$	$BO + N = BN + O$
$BOF + M = BF + O + M$	$BO + O = B + O_2$
$BOCl + M = BO + Cl + M$	$LO + BCl = B + BOCl$
$BClF + M = BCl + F + M$	$BO + BOCl = BO_2 + BCl$
$BCl_2F + M = BClF + Cl + M$	$BO + BF = B + BOF$
$BClF_2 + M = BF_2 + Cl + M$	$BOF + BF_2 = BF_3 + BO$
$BClF_2 + M = BClF + F + M$	$BO + BOF = BF + BO_2$
$B + N_2 = BN + N$	$BO_2 + HF = BOF + OH$
$B + NO = BN + O$	$BO_2 + Cl = BOCl + O$
$N + BO = NO + B$	$BO_2 + H = BO + OH$
$N_2 + BO = NO + BN$	$BO_2 + O = BO + O_2$

Table V. (continued)

<u>Chemical Reaction</u>	<u>Chemical Reaction</u>
$BCl + BCl = B + BCl_2$	$BF + BF_2 = B + BF_3$
$BCl + Cl = B + Cl_2$	$BF + BOF = BO + BF_2$
$BCl + H = B + HCl$	$BF_2 + F = BF + F_2$
$BCl + N = BN + Cl$	$BF_3 + F = BF_2 + F_2$
$BCl + BOF = BOCl + BF$	$BF_3 + H = BF_2 + HF$
$BCl_2 + Cl = BCl + Cl_2$	$BOF + BOF = BO_2 + BF_2$
$BCl_3 + Cl = BCl_2 + Cl_2$	$BOF + HCl = BOCl + HF$
$BOCl + HCl = BCl_2 + OH$	$BOF + HF = BF_2 + OH$
$HCl + SO_2 = OH + BOCl$	$BOF + Cl = BOCl + F$
$BOCl + Cl = BO + Cl_2$	$BOF + F = BO + F_2$
$BOCl + Cl = BCl_2 + O$	$BOF + F = BF_2 + O$
$BOCl + H = BO + HCl$	$BOF + H = BO + HF$
$BOCl + H = BCl + OH$	$BOF + H = BF + OH$
$BOCl + N = BCl + NO$	$BOF + O = BO_2 + F$
$BOCl + O = BCl + O_2$	$F + BCl = ClF + B$
$BF + BF = B + BF_2$	$B + CN = BN + C$
$CO + BOF = CO_2 + BF$	$C + BF = CF + B$
$BF + CO = BOF + C$	$B + HCN = BN + CH$
$BF + HCl = BCl + HF$	$CN + BF = CNF + B$
$BF + HF = BF_2 + H$	$B + CNF = BN + CF$
$BF + Cl = BCl + F$	$CN + BCl = CNCl + B$
$BF + F = B + F_2$	$BCl + BCl_2 = BCl_3 + B$
$BF + H = B + HF$	$BF + BCl = BClF + B$
$BF + N = BN + F$	$BCl + BClF = BCl_2F + B$

Table V. (continued)

<u>Chemical Reaction</u>	<u>Chemical Reaction</u>
$BF + BCl_2 = BCl_2F + B$	$C + BF_2 = CF + BF$
$BCl + BF_2 = BClF_2 + B$	$BF + CNF = BF_2 + CN$
$CN + BO = CO + BN$	$BF + CNCl = BCl + CNF$
$CN + BF = CF + BN$	$BF + CNCl = BCIF + CN$
$F + BOCI = ClF + BO$	$BF + BCl_2 = BCIF + BCl$
$CO + BF = CF + BO$	$BF + BCl_3 = BCl_2 + BCIF$
$C + BOF = CF + BO$	$BF + BCIF = BCl + BF_2$
$CN + BOCI = CNCl + BO$	$BF + BCl_2F = BCl + BCIF_2$
$BCl + BOCI = BCl_2 + BO$	$BF + BCl_2F = BCl_2 + BF_2$
$BCl_2 + BOCI = BCl_3 + BO$	$BF + BCl_2F = BCIF + BCIF$
$BF + BOCI = BCIF + BO$	$BF + BCIF_2 = BCl + BF_3$
$BCl + BOF = BCIF + BO$	$BF + BCIF_2 = BCIF + BF_2$
$BCl_2 + BOF = BCl_2F + BO$	$BF_2 + Cl = BCIF + F$
$BCIF + BOCI = BCl_2F + BO$	$BF_2 + Cl_2 = BCIF + ClF$
$BO + BCIF_2 = BOCI + BF_2$	$Cl + BCIF_2 = Cl_2 + BF_2$
$BCIF + BOF = BCIF_2 + BO$	$BF_2 + HCl = BCIF + HF$
$CO + BOF = CF + BO_2$	$BCIF_2 + H = HCl + BF_2$
$BOCl + BOCI = BCl_2 + BO_2$	$Cl + BF_3 = ClF + BF_2$
$BOF + BOCI = BCIF + BO_2$	$BF_2 + ClF = F_2 + BCIF$
$BF + Cl_2 = BCl + ClF$	$F + BCIF_2 = ClF + BF_2$
$Cl + BCIF = Cl_2 + BF$	$CO + BF_2 = CF + BOF$
$BF + HCl = BCIF + H$	$BF_2 + CNCl = BCIF + CNF$
$F + BCIF = ClF + BF$	$C + BF_3 = CF + BF_2$
$BF + ClF = BCl + F_2$	$CN + BF_3 = CNF + BF_2$

Table V. (continued)

<u>Chemical Reaction</u>	<u>Chemical Reaction</u>
$CN + BCIF_2 = CNCI + BF_2$	$BOF + BCl_2 = BOCl + BCIF$
$BCIF_2 + BCl = BCl_2 + BF_2$	$BOF + BCl_3 = BOCl + BCl_2F$
$BF_2 + BCl_2 = BCIF + BCIF$	$BOF + BCl_2F = BOCl + BCIF_2$
$BCIF_2 + BCl_2 = BCl_3 + BF_2$	$F + BCIF = F_2 + BCl$
$BCl_2F + BCIF = BF_2 + BCl_3$	$BCl + HF = BCIF + H$
$BCIF + BOF = BOCl + BF_2$	$BCl + HCl = BCl_2 + H$
$BF_3 + BCl = BCIF + BF_2$	$F + BCl_2 = ClF + BCl$
$BF_3 + BCl_2 = BCl_2F + BF_2$	$Cl + BCIF = ClF + BCl$
$BCIF_2 + BCIF = BCl_2F + BF_2$	$CO + BOCl = CO_2 + BCl$
$BF_3 + BCIF = BCIF_2 + BF_2$	$C + BCIF = CF + BCl$
$BF_3 + Cl = BCIF_2 + F$	$BCl + CNF = BCIF + CN$
$BF_3 + Cl_2 = BCIF_2 + ClF$	$BCl + CNCI = BCl_2 + CN$
$BF_3 + HCl = BCIF_2 + HF$	$BCl + BCl_3 = BCl_2 + BCl_2$
$BF_3 + ClF = BCIF_2 + F_2$	$BCl + BCl_2F = BCl_2 + BCIF$
$BF_3 + CNCI = BCIF_2 + CNF$	$BCl + BCIF_2 = BCIF + BCIF$
$BF_3 + BCl_2 = BCIF + BCIF_2$	$Cl + BCIF = F + BCl_2$
$BF_3 + BCl_3 = BCl_2F + BCIF_2$	$ClF + BCIF = F_2 + BCl_2$
$BCIF_2 + BOF = BOCl + BF_3$	$F + BCl_2F = F_2 + BCl_2$
$BF_3 + BCl_2F = BCIF_2 + BCIF_2$	$Cl + BCIF_2 = F_2 + BCl_2$
$BOF + Cl = BCIF + O$	$HCl + BCIF = HF + BCl_2$
$BOF + Cl_2 = BOCl + ClF$	$H + BCl_2F = HF + BCl_2$
$BOF + HCl = BCIF + OH$	$H + BCl_3 = HCl + BCl_2$
$BOF + ClF = BOCl + F_2$	$F + BCl_3 = ClF + BCl_2$
$BOF + CNCI = BOCl + CNF$	$Cl_2 + BCIF = ClF + BCl_2$

Table V. (continued)

<u>Chemical Reaction</u>	<u>Chemical Reaction</u>
$\text{Cl} + \text{BCl}_2\text{F} = \text{ClF} + \text{BCl}_2$	$\text{Cl} + \text{BCl}_2\text{F} = \text{Cl}_2 + \text{BClF}$
$\text{C} + \text{BCl}_2\text{F} = \text{CF} + \text{BCl}_2$	$\text{F} + \text{BClF}_2 = \text{F}_2 + \text{BClF}$
$\text{CNCl} + 3\text{ClF} = \text{CNF} + \text{BCl}_2$	$\text{H} + \text{BClF}_2 = \text{HF} + \text{BClF}$
$\text{CN} + \text{BCl}_2\text{F} = \text{CNF} + \text{BCl}_2$	$\text{H} + \text{BCl}_2\text{F} = \text{HCl} + \text{BClF}$
$\text{BCl}_2 + \text{CNCl} = \text{BCl}_3 + \text{CN}$	$\text{F} + \text{BCl}_2\text{F} = \text{ClF} + \text{BClF}$
$\text{BCl}_2 + \text{BClF}_2 = \text{BClF} + \text{BCl}_2\text{F}$	$\text{Cl} + \text{BClF}_2 = \text{ClF} + \text{BClF}$
$\text{Cl} + \text{BCl}_2\text{F} = \text{F} + \text{BCl}_3$	$\text{C} + \text{BClF}_2 = \text{CF} + \text{BClF}$
$\text{ClF} + \text{BCl}_2\text{F} = \text{F}_2 + \text{BCl}_3$	$\text{CN} + \text{BClF}_2 = \text{CNF} + \text{BClF}$
$\text{BCl}_2 + \text{BCl}_2\text{F} = \text{BCl}_3 + \text{BClF}$	$\text{CN} + \text{BCl}_2\text{F} = \text{CNCl} + \text{BClF}$
$\text{HCl} + \text{BCl}_2\text{F} = \text{HF} + \text{BCl}_3$	$\text{Cl} + \text{BClF}_2 = \text{F} + \text{BCl}_2\text{F}$
$\text{Cl}_2 + \text{BCl}_2\text{F} = \text{ClF} + \text{BCl}_3$	$\text{HCl} + \text{BClF}_2 = \text{HF} + \text{BCl}_2\text{F}$
$\text{CNCl} + \text{BCl}_2\text{F} = \text{CNF} + \text{BCl}_3$	$\text{Cl}_2 + \text{BClF}_2 = \text{ClF} + \text{BCl}_2\text{F}$
$\text{BCl}_2\text{F} + \text{BCl}_2\text{F} = \text{BClF}_2 + \text{BCl}_3$	$\text{CNCl} + \text{BClF}_2 = \text{CNF} + \text{BCl}_2\text{F}$
$\text{BOCl} + \text{F} = \text{BClF} + \text{O}$	$\text{ClF} + \text{BClF}_2 = \text{F}_2 + \text{BCl}_2\text{F}$
$\text{BOCl} + \text{HF} = \text{BClF} + \text{OH}$	$\text{BCl} + \text{CO} = \text{BOCl} + \text{C}$
$\text{CO} + \text{BClF} = \text{CF} + \text{BOCl}$	

Table VI. Additional Chemical Reactions of Importance in Lithium Containing Propellant Systems

<u>Chemical Reaction</u>	<u>Chemical Reaction</u>
$\text{LiH} + \text{M} = \text{Li} + \text{H} + \text{M}$	$\text{LiO} + \text{OH} = \text{LiH} + \text{O}_2$
$\text{LiOH} + \text{M} = \text{Li} + \text{OH} + \text{M}$	$\text{NO} + \text{Li} = \text{N} + \text{LiO}$
$\text{LiO} + \text{M} = \text{Li} + \text{O} + \text{M}$	$\text{LiO} + \text{LiOH} = \text{Li}_2\text{O} + \text{OH}$
$\text{Li}_2\text{O} + \text{M} = \text{Li} + \text{LiO} + \text{M}$	$\text{LiO} + \text{LiF} = \text{Li}_2\text{O} + \text{F}$
$\text{LiCl} + \text{M} = \text{Li} + \text{Cl} + \text{M}$	$\text{LiOH} + \text{LiOH} = \text{H}_2\text{O} + \text{Li}_2\text{O}$
$\text{Li}_2\text{Cl}_2 + \text{M} = \text{LiCl} + \text{LiCl} + \text{M}$	$\text{LiF} + \text{LiOH} = \text{HF} + \text{Li}_2\text{O}$
$\text{LiF} + \text{M} = \text{Li} + \text{F} + \text{M}$	$\text{Li}_2\text{O} + \text{H}_2 = \text{LiH} + \text{LiOH}$
$\text{Li}_2\text{F}_2 + \text{M} = \text{LiF} + \text{LiF} + \text{M}$	$\text{Li}_2\text{O} + \text{H} = \text{LiH} + \text{LiO}$
$\text{LiOH} + \text{M} = \text{LiO} + \text{H} + \text{M}$	$\text{Li}_2\text{O} + \text{O} = \text{LiO} + \text{LiO}$
$\text{Li} + \text{H}_2\text{O} = \text{LiH} + \text{OH}$	$\text{H}_2\text{O} + \text{LiCl} = \text{HCl} + \text{LiOH}$
$\text{Li} + \text{H}_2\text{O} = \text{LiOH} + \text{H}$	$\text{LiOH} + \text{H}_2 = \text{LiH} + \text{H}_2\text{O}$
$\text{Li} + \text{CO} = \text{LiO} + \text{C}$	$\text{LiOH} + \text{OH} = \text{LiO} + \text{H}_2\text{O}$
$\text{Li} + \text{HF} = \text{LiH} + \text{F}$	$\text{OH} + \text{LiCl} = \text{Cl} + \text{LiOH}$
$\text{Li} + \text{H}_2 = \text{LiH} + \text{H}$	$\text{LiOH} + \text{H} = \text{LiH} + \text{OH}$
$\text{Li} + \text{OH} = \text{LiH} + \text{O}$	$\text{LiOH} + \text{H} = \text{LiO} + \text{H}_2$
$\text{Li} + \text{OH} = \text{LiO} + \text{H}$	$\text{LiOH} + \text{O} = \text{LiO} + \text{OH}$
$\text{Li} + \text{O}_2 = \text{LiO} + \text{O}$	$\text{LiOH} + \text{LiCl} = \text{Li}_2\text{O} + \text{HCl}$
$\text{Li} + \text{LiOH} = \text{LiH} + \text{LiO}$	$\text{LiF} + \text{H}_2\text{O} = \text{LiOH} + \text{HF}$
$\text{Li} + \text{LiOH} = \text{Li}_2\text{O} + \text{H}$	$\text{LiF} + \text{HF} = \text{LiH} + \text{F}_2$
$\text{HCl} + \text{Li} = \text{Cl} + \text{LiH}$	$\text{LiF} + \text{H}_2 = \text{LiH} + \text{HF}$
$\text{CO}_2 + \text{Li} = \text{CO} + \text{LiO}$	$\text{LiF} + \text{OH} = \text{LiOH} + \text{F}$
$\text{Cl} + \text{LiOH} = \text{HCl} + \text{LiO}$	$\text{LiF} + \text{OH} = \text{LiO} + \text{HF}$
$\text{LiO} + \text{HF} = \text{LiOH} + \text{F}$	$\text{LiF} + \text{Cl} = \text{LiCl} + \text{F}$
$\text{LiO} + \text{H}_2 = \text{LiH} + \text{OH}$	$\text{LiF} + \text{F} = \text{Li} + \text{F}_2$

Table VI. (continued)

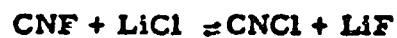
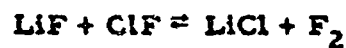
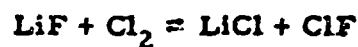
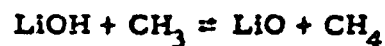
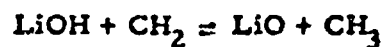
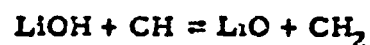
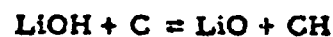
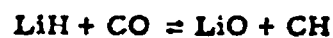
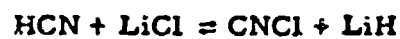
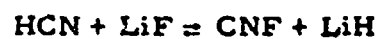
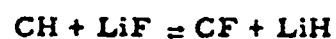
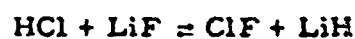
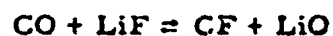
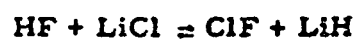
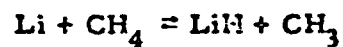
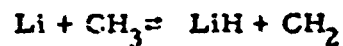
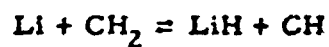
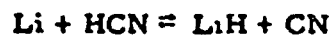
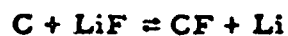
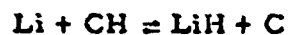
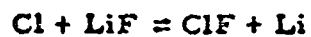
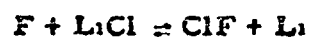
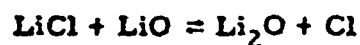
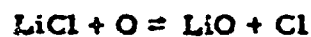
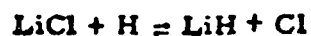
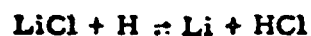
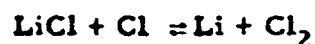
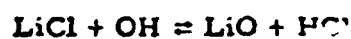
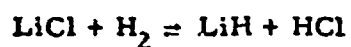
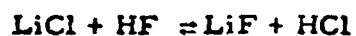
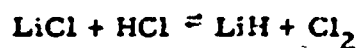
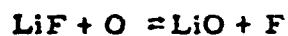
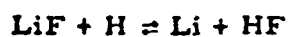
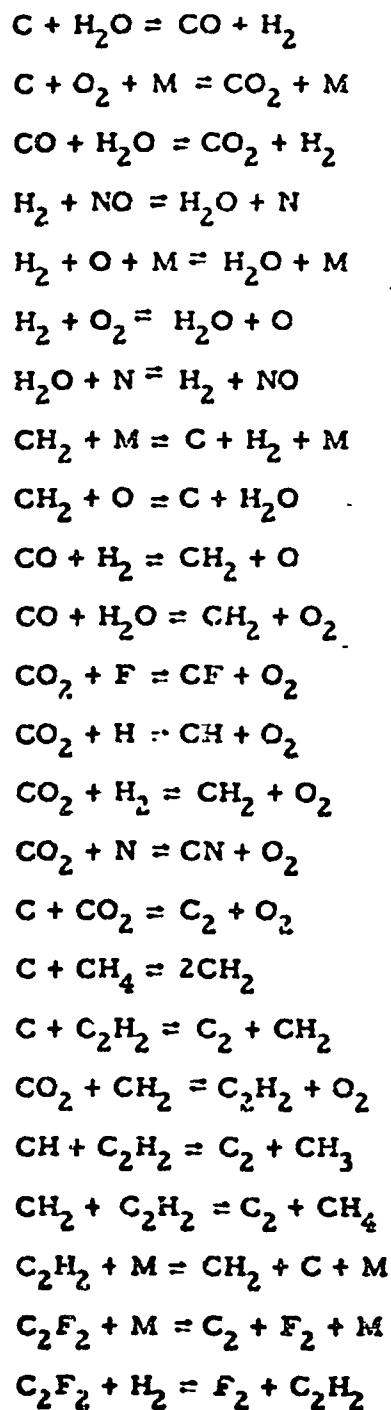


Table VII. Chemical Reactions Eliminated Due to Steric Considerations

Chemical Reactions Involving  
No Metallized Species



Chemical Reactions Involving  
No Metallized Species

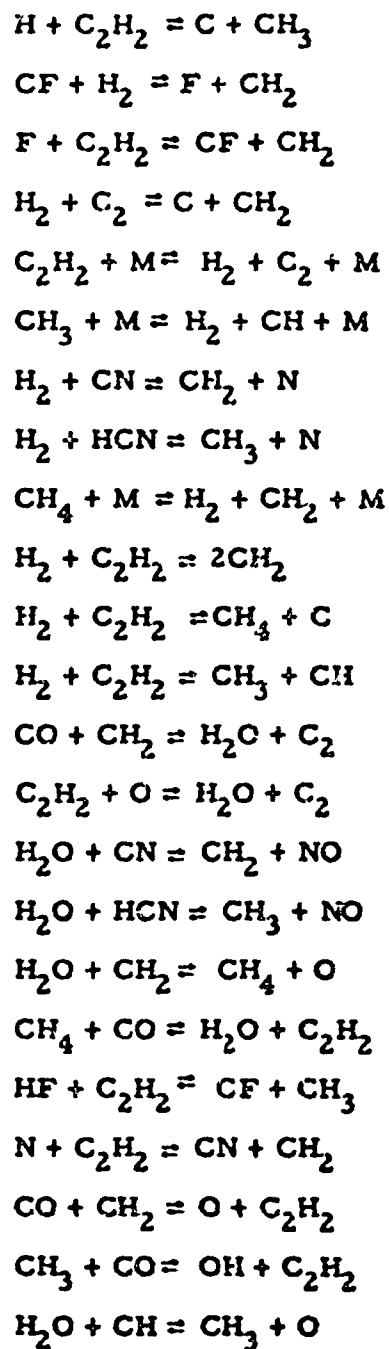
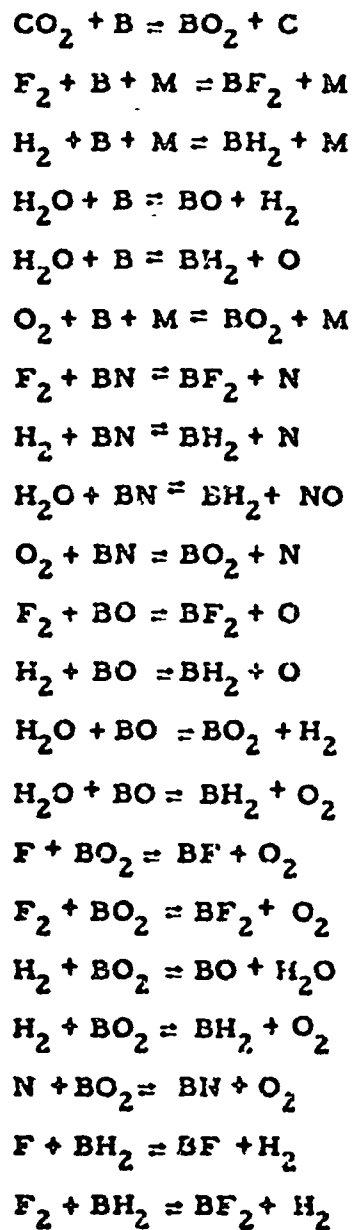




Table VII. (continued) Chemical Reactions Eliminated  
Due to Steric Considerations

Chemical Reactions involving  
Boron Species



Chemical Reactions Involving  
Boron Species (continued)

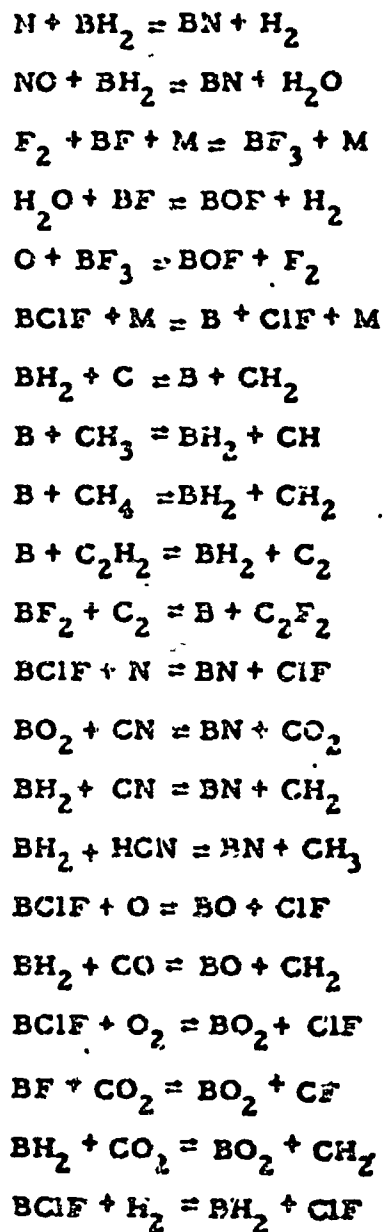
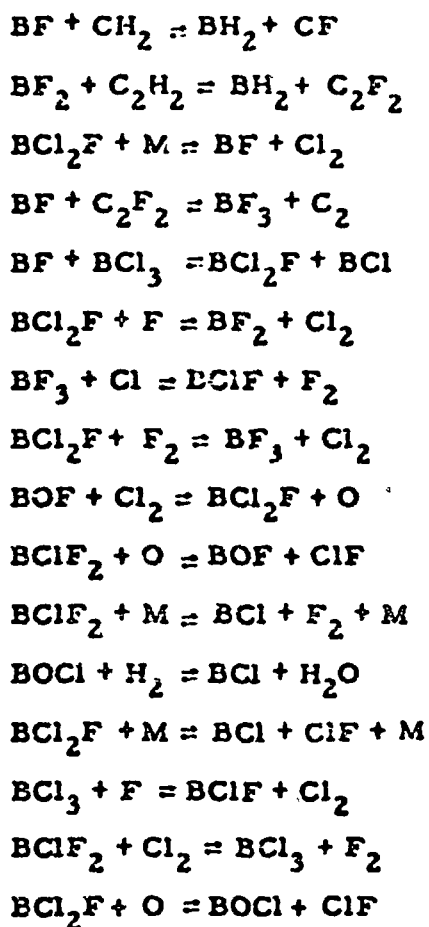
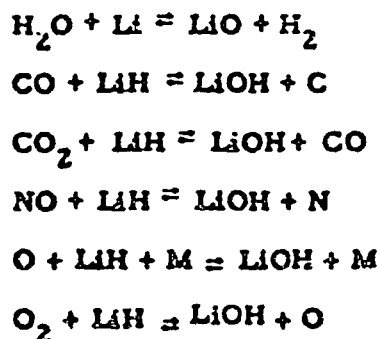


Table VII. (continued) Chemical Reactions Eliminated  
Due to Steric Considerations

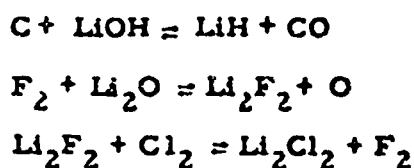
Chemical Reactions Involving  
Boron Species (Continued)



Chemical Reactions Involving  
Lithium Species



Chemical Reactions Involving  
Lithium Species (continued)



Chemical Reactions Involving  
Aluminum Species

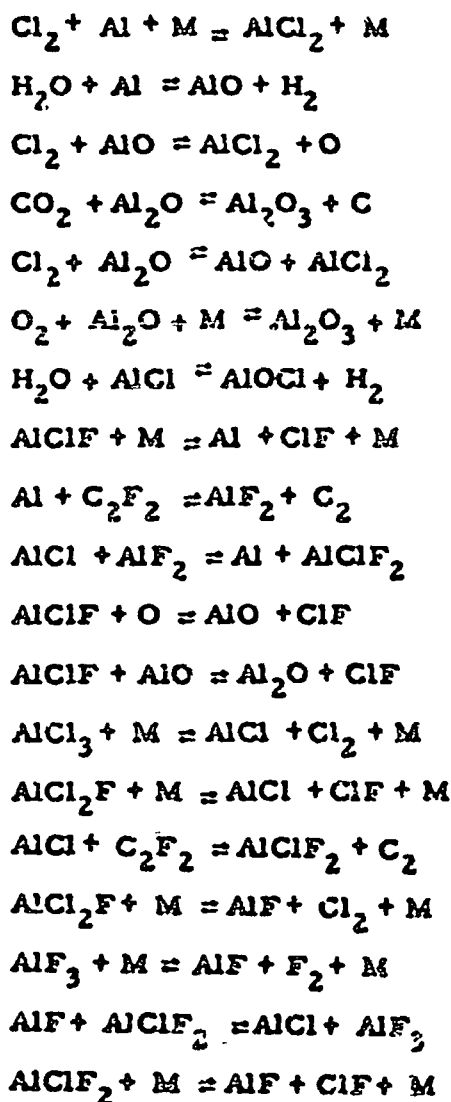
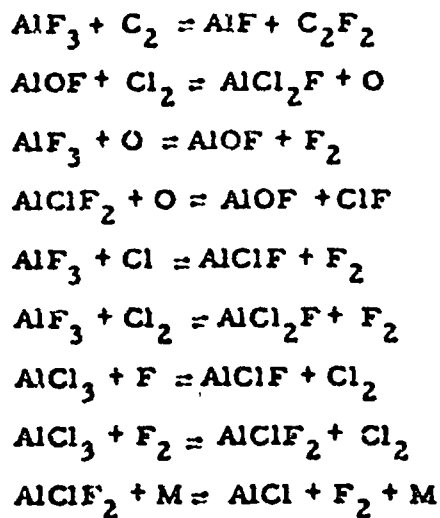


Table VII. (continued) Chemical Reactions Eliminated  
Due to Steric Considerations

Chemical Reactions Involving  
Aluminum Species (continued)



Chemical Reactions Involving  
Beryllium Species

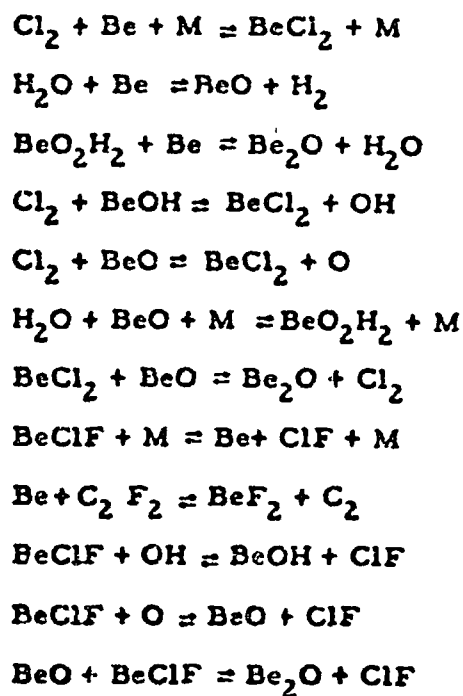


Table VIII. Spin Forbidden Chemical Reactions Which Do Not Occur In the Ground State

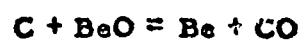
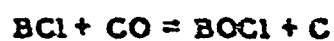
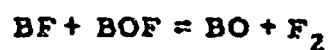
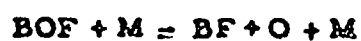
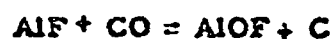
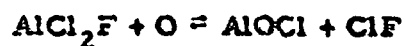
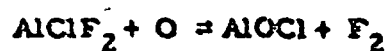
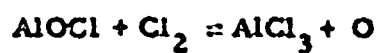
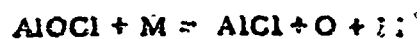
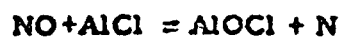
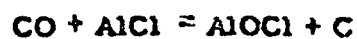
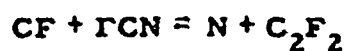
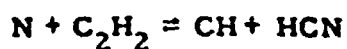
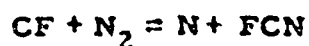
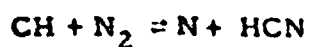
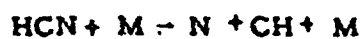
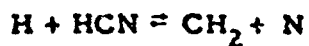
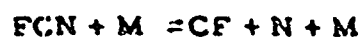
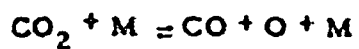


Table IX. Chemical Reactions for Which Rate Constants Have Been Determined

Chemical Reaction	Exothermic Rate Constant*	Reference
$\text{CO}_2 + \text{M} \rightleftharpoons \text{CO} + \text{O} + \text{M}$	$3 \times 10^{20} T^{-1.0} \exp \left( -\frac{11393}{T} \right)$	Avramenko, L. I. and Kolesnikova, R. V., Invest. Akad. Nauk. S.S.S.R., Otdel. Khim. Navh., 1962 (1959).
$\text{H}_2\text{O} + \text{M} \rightleftharpoons \text{OH} + \text{H} + \text{M}$	$3 \times 10^{19} T^{-1.0}$	Mayer, S. W., Cook, E. A., Schieler, L., "Nonequilibrium Recombination in Nozzles," SSD-TDR-64-139, Aerospace Corporation, Los Angeles, California, 18 Sept. 1964.
$\text{CO} + \text{M} \rightleftharpoons \text{C} + \text{O} + \text{M}$	$2 \times 10^{18} T^{-1.0}$	Wray, K. L., Avco Research Report 95 (1961).
$\text{HF} + \text{M} \rightleftharpoons \text{H} + \text{F} + \text{M}$	$1 \times 10^{19} \times T^{-0.5}$	S. W. Mayer, E. A. Cook, and L. Schieler, "Nonequilibrium Recombination in Nozzles," SSD-TDR-64-139, Aerospace Corporation, Los Angeles, California, 19 Sept. 1964.
$\text{H}_2 + \text{M} \rightleftharpoons 2\text{H} + \text{M}$	$10^{19} T^{-1.0}$	W. E. Kashan and W. G. Browne, "Kinetics of the H <sub>2</sub> /CO/O <sub>2</sub> System," General Electric Document No. 61SD848, 16 February 1964.
$\text{N}_2 + \text{M} \rightleftharpoons 2\text{N} + \text{M}$	$2 \times 10^{18} T^{-1.0}$	K. L. Wray, Avco Research Report 104 (1961).
$\text{NO} + \text{M} \rightleftharpoons \text{N} + \text{O} + \text{M}$	$2 \times 10^{18} T^{-1.0}$	K. L. Wray, Avco Research Report 95 (1961).
$\text{OH} + \text{M} \rightleftharpoons \text{O} + \text{H} + \text{M}$	$2 \times 10^{18} T^{-1.0}$	S. W. Mayer, E. A. Cook, and L. Schieler, "Nonequilibrium Recombination in Nozzles," SSD-TDR-64-139, Aerospace Corporation, Los Angeles, California, 19 Sept. 1964.
$\text{O}_2 + \text{M} \rightleftharpoons 2\text{O} + \text{M}$	$1 \times 10^{16} T^{-0.5}$	S. W. Mayer, E. A. Cook, and L. Schieler, "Nonequilibrium Recombination in Nozzles," SSD-TDR-64-139, Aerospace Corporation, Los Angeles, California, 19 Sept. 1964.
$\text{CO}_2 + \text{H}_2 \rightleftharpoons \text{CO} + \text{OH}$	$3.2 \times 10^{12} \exp \left( -\frac{6100}{RT} \right)$	W. E. Kashan and W. G. Browne, "Kinetics of the H <sub>2</sub> /CO/O <sub>2</sub> System," General Electric Document No. 61SD848, 16 Feb. 1964.
$\text{CO}_2 + \text{O} \rightleftharpoons \text{CO} + \text{O}_2$	$3.58 \times 10^{14} T^{-1.0}$	L. I. Avramenko and R. V. Kolesnikova, Invest. Akad. Nauk. S.S.S.R., Otdel. Khim. Navh., 1962 (1959).
$\text{H}_2\text{O} + \text{H} \rightleftharpoons \text{OH} + \text{H}_2$	$7 \times 10^{13} \exp \left( -\frac{6100}{RT} \right)$	S. W. Mayer, E. A. Cook, and L. Schieler, "Nonequilibrium Recombination in Nozzles," SSD-TDR-64-139, Aerospace Corporation, Los Angeles, California, 19 Sept. 1964.
$\text{H}_2\text{O} + \text{O} \rightleftharpoons 2\text{OH}$	$2.9 \times 10^{14} \exp \left( -\frac{10000}{RT} \right)$	S. W. Mayer, E. A. Cook, and L. Schieler, "Nonequilibrium Recombination in Nozzles," SSD-TDR-64-139, Aerospace Corporation, Los Angeles, California, 19 Sept. 1964.

\* Three body recombination rates have the units  $\text{cm}^6/\text{gmole}^2\text{-sec}$ .  
Bimolecular reaction rates have the units  $\text{cm}^3/\text{gmole-sec}$ .

Table IX. Chemical Reactions for Which Rate Constants Have Been Determined (Continued)

Chemical Reaction	Exothermic Rate Constant	Reference
$2\text{CO} \rightleftharpoons \text{CO}_2 + \text{C}$	$2.11 \times 10^{16} T^{-1.0}$	L. L. Avramenko, R. V. Lorentso, Zhur. Fiz. Khim., <u>24</u> , 207 (1950).
$\text{CO} + \text{H}_2 \rightleftharpoons \text{C} + \text{OH}$	$1 \times 10^{14} \exp - \frac{13000}{T}$	F. Kaufman and J. P. Kelso, J. Chem. Phys., <u>23</u> , 1072 (1955).
$\text{CO} + \text{N}_2 \rightleftharpoons \text{C} + \text{NO}$	$1.44 \times 10^{16} T^{-1.0}$	L. L. Avramenko and R. V. Lorentso, Zhur. Fiz. Khim., <u>24</u> , 207 (1950).
$\text{CO} + \text{NO} \rightleftharpoons \text{CO}_2 + \text{N}$	$2.47 \times 10^{15} T^{-1.0}$	L. L. Avramenko and R. V. Kilaanikova, Izvest. Akad. Nauk. S.S.S.R., Otdel. Khim. Nauk., 1562 (1959).
$\text{CO} + \text{O} \rightleftharpoons \text{C} + \text{O}_2$	$2.48 \times 10^{13} \exp - \frac{990}{T}$	L. L. Avramenko and R. V. Lorentso, Zhur. Fiz. Khim., <u>20</u> , 207 (1950).
$\text{HF} + \text{H}_2 \rightleftharpoons \text{H}_2 + \text{F}$	$5 \times 10^{12} \exp - \frac{5700}{RT}$	S. W. Meyer, E. A. Cook, and L. Schieler, "Nonequilibrium Recombination in Nozzles," ASD-TDR-64-139 Aerospace Corporation, Los Angeles, California, 18 Sept. 1964.
$\text{HF} + \text{O}_2 \rightleftharpoons \text{OH} + \text{F}$	$5 \times 10^{11} T^{0.5} \exp - \frac{6000}{RT}$	S. W. Meyer, E. A. Cook, and L. Schieler, "Nonequilibrium Recombination in Nozzles," ASD-TDR-64-139 Aerospace Corporation, Los Angeles, California, 18 Sept. 1964.
$\text{HF} + \text{OH} \rightleftharpoons \text{H}_2\text{O} + \text{F}$	$5 \times 10^{11} T^{0.5} \exp - \frac{7000}{RT}$	S. W. Meyer, E. A. Cook, and L. Schieler, "Nonequilibrium Recombination in Nozzles," ASD-TDR-64-139 Aerospace Corporation, Los Angeles, California, 18 Sept. 1964.
$\text{H}_2 + \text{O} \rightleftharpoons \text{OH} + \text{H}$	$1.4 \times 10^{12} \exp - \frac{5190}{RT}$	W. E. Haxhan and W. G. Browne, "Kinetics of the $\text{H}_2/\text{CO}/\text{O}_2$ System," General Electric Document No. 6X1240, 16 February 1964.
$\text{H}_2 + \text{O}_2 \rightleftharpoons 2\text{OH}$	$2.7 \times 10^{16} \exp - \frac{13000}{T}$	F. Kaufman and J. P. Kelso, J. Chem. Phys., <u>23</u> , 1072 (1955).
$\text{N}_2 + \text{O} \rightleftharpoons \text{NO} + \text{N}$	$1.5 \times 10^{16} T^{-1}$	L. E. Phillips and H. I. Schiff, J. Chem. Phys., <u>16</u> , 1409 (1948).
$\text{N}_2 + \text{O}_2 \rightleftharpoons 2\text{NO}$	$9 \times 10^{23} T^{-3/2} \exp - \frac{42000}{T}$	E. Frostman and J. W. Damber, J. Chem. Phys., <u>16</u> , 1271 (1948).
$\text{NO} + \text{O} \rightleftharpoons \text{N} + \text{O}_2$	$1.011 \times 10^{11} T^{0.5} \exp - \frac{3120}{T}$	W. G. Vincenti, Stanford Univ. Dept. Aeronaut. Engr. Rept. 101 (1961).
$\text{O}_2 + \text{H}_2 \rightleftharpoons \text{OH} + \text{O}$	$3.2 \times 10^{11} T^{-0.47} \exp - \frac{100}{RT}$	W. E. Haxhan and W. G. Browne, "Kinetics of the $\text{H}_2/\text{CO}/\text{O}_2$ System," General Electric Document No. 6X1240, 16 Feb. 1964.