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

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Prepared for
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MANNED SPACECRAFT CENTER
Under
CONTRACT NAS9-4358

TRW SYSTEMS
One Space Park • Redondo Beach, California

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CONTENTS

1. 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, Development of Six (6) Computer Programs for Analytical Predictions of Delivered Specific Impulse.

The objective of this contract is to develop a family of six computer programs to calculate inviscid, one-dimensional and axisymmetric nonequilibrium nozzle flow fields. Assuming that equilibrium conditions exist in the combustion chamber, these programs will calculate the nonequilibrium nozzle expansion of propellant exhaust mixtures containing the elements: carbon, hydrogen, oxygen, nitrogen, fluorine, chlorine; and one metal element, either aluminum, beryllium, boron or lithium. These computer programs will account 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 chemical study described in this report was performed to determine the significant chemical species and chemical reactions in typical propellant exhaust mixtures containing the above elements for consideration in nonequilibrium performance calculations. The significant chemical species are 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 non-equilibrium flows having finite reaction rates. Thus, an additional restriction was imposed on the significant chemical species selection. The significant chemical species were defined for the purpose of this study 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.

After determining the significant species, all possible dissociation-recombination and binary exchange reactions between these species were studied. 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 and 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.

These studies are described in the following sections.

2. CHEMICAL SPECIES STUDY

A number of propellant systems containing the six 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 propellant. The propellant systems selected for study are given in Table I. 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 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^{-2} 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. Those significant species present in each propellant system studied are given in Table III. Comparisons of the equilibrium and frozen performance calculated considering all species present and only the significant species present is given in Tables IV through XVIII for all propellant systems studied.

Examination of Tables IV through XVIII 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 0.04 second of specific impulse at an area ratio of 40. This difference occurs in the frozen performance calculation of the monomethyl hydrazine-perchloryl fluoride system at a mixture ratio of 2.1 and 1000 psia chamber pressure. In the metallized systems, the maximum performance difference is 0.39 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 nonequilibrium 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 XIX through XXIII 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 XXIV) 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 procludes 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 program being 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 XIX through XXIII. Those reactions for which rates have been measured are given in Table XXVI. 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 XXV. Order of magnitude rate estimates can be obtained by statistical mechanics and kinetic theory for those reactions for which experimental rate data does not exist. The reaction rates for the "spin forbidden" reactions can be similarly estimated if the rate estimates are corrected by Boltzmann factors for the fact that these reactions do not occur in the ground state.

TABLES

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

	Fuel/Oxidizer	Mixture Ratios
1.	Hydrogen/Oxygen	MR = 5.0 ± 1.0
2.	Hydrogen/Fluorine	MR = 10.0 ± 3.0
3.	RP-1/Oxygen	MR = 2.6 ± 0.4
4.	Hydrazine/Nitrogen Tetroxide	MR = 1.1 ± 0.2
5.	Hydrazine/Compound "A"	MR = 2.5 ± 0.2
6.	Monomethyl Hydrazine/Nitrogen Tetroxide	MR = 1.8 ± 0.3
7.	Monomethyl Hydrazine/Oxygen Difluoride	MR = 1.8 ± 0.3
8.	Monomethyl Hydrazine/Perchloryl Fluoride	MR = 1.8 ± 0.3
9.	Diborane/Hydrazine	MR = 1.25 ± 0.1
10.	Diborane/Oxygen Difluoride	MR = 3.2 ± 0.8
11.	Lithium Hydride/Oxygen Difluoride	MR = 3.0 ± 0.5

	Fuel/Oxidizer	Composition
12.	PBAA—Aluminum/Ammonium Perchlorate	14 percent PBAA, 16 percent Al, 70 percent NH_4ClO_4
13.	PBAA—Beryllium/Ammonium Perchlorate	16 percent PBAA, 13 percent Be, 71 percent NH_4ClO_4
14.	Double Base—Aluminum/Ammonium Perchlorate	28.8 percent NG, 21.6 percent NC, 10.8 percent HMX, 19.8 Al, 10.8 percent NH_4ClO_4
15.	Double Base—Beryllium/Ammonium Perchlorate	32.4 percent NG, 15.0 percent NC, 29.0 percent HMX, 10.0 percent Be, 9.0 percent NH_4ClO_4, 4.6 percent Additives

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

Non-Metallized Species

C	F_2	N
CO	H	N_2
CO_2	H_2	NO
Cl	H_2O	O
Cl_2	HF	O_2
F	HCl	OH

Metallized Species

Al	Be	B	Li
AlO	BeOH	B(l)	LiH
Al_2O	BeO_2H_2	B(S)	LiOH
AlCl	BeO	BN	LiO
$AlCl_2$	BeO(l)	BN(S)	Li_2O
AlOCl	BeO(S)	BO	LiF
Al_2O_3	BeCl	BO_2	Li_2F_2
Al_2O_3(l)	$BeCl_2$	BH_2	
Al_2O_3(S)	Be_2O	BF	
		BF_2	
		BF_3	
		BOF	

Table III. Significant Species Considered in Each Propellant System

Propellant System (Table I)	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
Species															
C			X			X	X	X				X	X	X	X
CO			X			X	X	X				X	X	X	X
CO_2			X			X	X	X				X	X	X	X
Cl					X			X				X	X	X	X
Cl_2					X			X				X	X	X	X
F		X			X		X	X		X	X				
F_2		X			X		X	X		X	X				
H	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
H_2	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
H_2O	X		X	X		X	X	X		X	X	X	X	X	X
HF		X			X		X	X		X	X				
HCl					X			X				X	X	X	X
N				X	X	X	X	X	X			X	X	X	X
N_2				X	X	X	X	X	X			X	X	X	X
NO				X		X	X	X				X	X	X	X
O	X		X	X		X	X	X		X	X	X	X	X	X
O_2	X		X	X		X	X	X		X	X	X	X	X	X
OH	X		X	X		X	X	X		X	X	X	X	X	X
Al												X		X	
AlO												X		X	
Al_2O												X		X	
AlCl												X		X	

Table III. Significant Species Considered in Each Propellant System (Continued)

Propellant System (Table I)	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
Species															
$AlCl_2$												X		X	
AlOCl												X		X	
Al_2O_3												X		X	
Al_2O_3(l)												X		X	
Al_2O_3(S)												X		X	
Be													X		X
BeOH													X		X
BeO_2H_2													X		X
BeO													X		X
BeO(l)													X		X
BeO(S)													X		X
BeCl													X		X
$BeCl_2$													X		X
Be_2O													X		X
B									X	X					
B(l)									X	X					
B(S)									X	X					
BN									X						
BN(S)									X						
BO										X					
BO_2										X					
BH_2									X	X					

Table III. Significant Species Considered in Each Propellant System (Continued)

Propellant System (Table I)	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
Species															
BF										X					
BF_2										X					
BF_3										X					
BOF										X					
Li											X				
LiH											X				
LiOH											X				
LiO											X				
Li_2O											X				
LiF											X				
Li_2F_2											X				
Total Number of Species Considered in Each System	6	5	9	9	10	12	15	18	10	19	16	24	24	24	24

Table IV. Theoretical Performance of H_2/O_2 System

Chamber Pressure (psia)	Mixture Ratio	Area Ratio	I_{sp} (VAC) Equilibrium Flow: All Species	I_{sp} (VAC) Equilibrium Flow: 6 Significant Species	I_{sp} (VAC) Frozen Flow: All Species	I_{sp} (VAC) Frozen Flow: 6 Significant Species
100	4.0	10.0	425.99	425.99	415.04	415.04
		20.0	442.84	442.84	430.36	430.36
		30.0	450.70	450.70	437.48	437.48
		40.0	455.55	455.55	441.87	441.87
	5.0	10.0	421.42	421.42	402.37	402.37
		20.0	440.51	440.51	418.04	418.04
		30.0	449.67	449.67	425.39	425.39
		40.0	455.40	455.40	429.93	429.93
	6.0	10.0	412.08	412.08	387.58	387.58
		20.0	433.09	433.09	403.10	403.10
		30.0	443.41	443.41	410.43	410.43
		40.0	449.98	449.98	414.97	414.98
1000	4.0	10.0	427.01	427.01	422.02	422.02
		20.0	443.60	443.60	437.95	437.95
		30.0	451.35	451.35	445.37	445.37
		40.0	456.13	456.13	449.95	449.95
	5.0	10.0	424.36	424.36	413.55	413.55
		20.0	442.80	442.81	430.25	430.25
		30.0	451.66	451.66	438.15	438.15
		40.0	457.19	457.19	443.06	443.06
	6.0	10.0	417.72	417.72	401.19	401.19
		20.0	437.68	437.68	417.96	417.97
		30.0	447.46	447.46	425.99	426.00
		40.0	453.68	453.68	431.01	431.02

Table V. Theoretical Performance of H_2/F_2 System

Chamber Pressure (psia)	Mixture Ratio	Area Ratio	Isp (VAC) Equilibrium Flow: All Species	Isp (VAC) Equilibrium Flow: 5 Significant Species	Isp (VAC) Frozen Flow: All Species	Isp (VAC) Frozen Flow: 5 Significant Species
100	7.0	10.0	443.93	443.93	410.49	410.49
		20.0	460.76	460.76	421.97	421.97
		30.0	468.33	468.33	427.10	427.10
		40.0	472.87	472.87	430.22	430.22
	10.0	10.0	439.15	439.15	397.12	397.12
		20.0	458.94	458.94	407.91	407.91
		30.0	468.23	468.23	412.68	412.68
		40.0	473.92	473.92	415.56	415.56
	13.0	10.0	433.94	433.94	387.44	387.44
		20.0	454.89	454.89	397.75	397.75
		30.0	465.13	465.13	402.28	402.28
		40.0	471.57	471.57	405.00	405.00
1000	7.0	10.0	448.06	448.06	426.87	426.87
		20.0	463.74	463.74	439.46	439.46
		30.0	470.78	470.78	445.06	445.06
		40.0	475.01	475.01	448.45	448.45
	10.0	10.0	447.25	447.25	416.27	416.27
		20.0	465.21	465.21	428.40	428.40
		30.0	473.51	473.51	433.75	433.76
		40.0	478.57	478.57	436.97	436.97
	13.0	10.0	444.18	444.18	407.19	407.19
		20.0	463.58	463.58	418.88	418.88
		30.0	472.74	472.74	424.01	424.02
		40.0	478.41	478.41	427.08	427.10

Table VI. Theoretical Performance of RP-1/O_2 System

Chamber Pressure (psia)	Mixture Ratio	Area Ratio	I_{sp} (VAC) Equilibrium Flow All Species	I_{sp} (VAC) Equilibrium Flow 9 Significant Species	I_{sp} (VAC) Frozen Flow All Species	I_{sp} (VAC) Frozen Flow 9 Significant Species
100	2.2	10.0	320.10	320.10	301.61	301.62
		20.0	335.14	335.14	313.17	313.18
		30.0	342.49	342.49	318.61	318.62
		40.0	347.17	347.17	321.98	321.99
	2.6	10.0	320.65	320.65	297.29	297.30
		20.0	338.29	338.29	309.03	309.04
		30.0	347.17	347.18	314.60	314.60
		40.0	352.91	352.91	318.06	318.07
	3.0	10.0	315.06	315.07	291.40	291.40
		20.0	333.32	333.32	303.08	303.08
		30.0	342.84	342.84	308.65	308.65
		40.0	349.15	349.16	312.11	312.12
1000	2.2	10.0	323.22	323.22	311.55	311.57
		20.0	337.63	337.63	323.94	323.96
		30.0	344.68	344.69	329.83	329.85
		40.0	349.18	349.18	333.49	333.52
	2.6	10.0	327.31	327.32	309.12	309.14
		20.0	344.08	344.09	321.85	321.88
		30.0	352.41	352.41	327.97	328.00
		40.0	357.75	357.76	331.82	331.84
	3.0	10.0	323.21	323.22	303.46	303.48
		20.0	341.38	341.39	316.16	316.18
		30.0	350.77	350.77	322.29	322.32
		40.0	356.94	356.94	326.16	326.18

Table VII. Theoretical Performance of N_2H_4/N_2O_4 System

Chamber Pressure (psia)	Mixture Ratio	Area Ratio	I_{sp} (VAC) Equilibrium Flow: All Species	Equilibrium Flow: 9 Significant Species	Frozen Flow: All Species	Frozen Flow: 9 Significant Species
100	0.9	10.0	310.06	310.06	303.11	303.12
		20.0	321.77	321.77	314.00	314.00
		30.0	327.22	327.22	319.05	319.05
		40.0	330.58	330.58	322.16	322.17
	1.1	10.0	314.68	314.68	302.44	302.44
		20.0	327.65	327.65	313.68	313.68
		30.0	333.76	333.76	318.91	318.92
		40.0	337.55	337.55	322.15	322.15
	1.3	10.0	315.95	315.95	298.38	298.38
		20.0	330.24	330.24	309.65	309.65
		30.0	337.08	337.08	314.92	314.92
		40.0	341.35	341.35	318.18	318.18
1000	0.9	10.0	310.57	310.58	307.54	307.55
		20.0	322.16	322.16	318.78	318.78
		30.0	327.55	327.55	324.00	324.00
		40.0	330.87	330.87	327.22	327.23
	1.1	10.0	315.96	315.96	309.48	309.49
		20.0	328.62	328.62	321.31	321.31
		30.0	334.59	334.59	326.84	326.85
		40.0	338.29	338.29	330.27	330.28
	1.3	10.0	318.45	318.44	307.01	307.01
		20.0	332.18	332.19	319.01	319.02
		30.0	338.75	338.75	324.66	324.67
		40.0	342.85	342.85	328.17	328.18

Table VIII. Theoretical Performance of N_2H_4/Compound A System

Chamber Pressure (psia)	Mixture Ratio	Area Ratio	I_{sp} (VAC) Equilibrium Flow: All Species	I_{sp} (VAC) Equilibrium Flow: 10 Significant Species	I_{sp} (VAC) Frozen Flow: All Species	I_{sp} (VAC) Frozen Flow: 10 Significant Species
100	2.3	10.0	340.94	340.94	311.55	311.56
		20.0	355.27	355.27	320.42	320.43
		30.0	361.89	361.89	324.37	324.38
		40.0	365.92	365.92	326.76	326.77
	2.5	10.0	341.63	341.63	312.42	312.43
		20.0	356.48	356.48	321.37	321.38
		30.0	363.42	363.42	325.36	325.37
		40.0	367.65	367.65	327.78	327.79
	2.7	10.0	341.59	341.60	310.25	310.26
		20.0	356.86	356.86	319.02	319.04
		30.0	364.12	364.12	322.93	322.94
		40.0	368.60	368.60	325.29	325.30
1000	2.3	10.0	345.52	345.53	325.22	325.24
		20.0	358.71	358.71	335.06	335.08
		30.0	364.77	364.77	339.45	339.48
		40.0	368.46	368.46	342.11	342.14
	2.5	10.0	346.79	346.79	324.51	324.53
		20.0	360.43	360.43	334.27	334.30
		30.0	366.73	366.74	338.63	338.66
		40.0	370.58	370.58	341.26	341.29
	2.7	10.0	347.16	347.17	323.22	323.25
		20.0	361.31	361.31	332.87	332.91
		30.0	367.92	367.92	337.18	337.21
		40.0	371.96	371.97	339.78	339.81

Table IX. Theoretical Performance of MMH/N_2O_4 System

Chamber Pressure (psia)	Mixture Ratio	Area Ratio	I_{sp} (VAC) Equilibrium Flow All Species	I_{sp} (VAC) Equilibrium Flow 12 Significant Species	I_{sp} (VAC) Frozen Flow All Species	I_{sp} (VAC) Frozen Flow 12 Significant Species
100	1.5	10.0	304.66	304.66	295.75	295.76
		20.0	316.84	316.84	306.45	306.45
		30.0	322.68	322.68	311.42	311.43
		40.0	326.36	326.36	314.49	314.50
	1.8	10.0	309.86	309.86	294.84	294.85
		20.0	323.42	323.42	305.92	305.92
		30.0	329.95	329.95	311.10	311.11
		40.0	334.07	334.07	314.31	314.31
	2.1	10.0	310.76	310.76	290.57	290.57
		20.0	325.85	325.85	301.70	301.70
		30.0	333.18	333.18	306.92	306.93
		40.0	337.83	337.83	310.16	310.17
1000	1.5	10.0	305.38	305.38	300.95	300.96
		20.0	317.40	317.40	312.06	312.07
		30.0	323.17	323.17	317.24	317.25
		40.0	326.81	326.81	320.44	320.45
	1.8	10.0	311.71	311.71	302.90	302.91
		20.0	324.86	324.87	314.64	314.66
		30.0	331.21	331.21	320.17	320.19
		40.0	335.21	335.21	323.60	323.62
	2.1	10.0	314.28	314.28	300.03	300.04
		20.0	328.64	328.64	311.95	311.97
		30.0	335.63	335.63	317.61	317.62
		40.0	340.06	340.06	321.13	321.14

Table X. Theoretical Performance of MMH/OF_2 System

Chamber Pressure (psia)	Mixture Ratio	Area Ratio	I_{sp} (VAC) Equilibrium Flow All Species	Equilibrium Flow 15 Significant Species	Frozen Flow All Species	Frozen Flow 15 Significant Species
100	1.5	10.0	357.82	357.82	333.68	333.68
		20.0	371.75	371.75	343.74	343.75
		30.0	378.16	378.16	348.27	348.28
		40.0	382.07	382.07	351.03	351.03
	1.8	10.0	364.08	364.08	333.69	333.70
		20.0	379.97	379.98	343.78	343.79
		30.0	387.43	387.43	348.32	348.32
		40.0	392.03	392.03	351.07	351.07
	2.1	10.0	366.18	366.19	331.65	331.65
		20.0	383.86	383.86	341.63	341.64
		30.0	392.34	392.34	346.10	346.11
		40.0	397.62	397.62	348.82	348.83
1000	1.5	10.0	360.88	360.88	345.85	345.88
		20.0	374.01	374.02	356.83	356.83
		30.0	380.06	380.06	361.76	361.76
		40.0	383.76	383.76	364.75	364.75
	1.8	10.0	369.15	369.15	347.86	347.89
		20.0	383.83	383.84	359.00	359.03
		30.0	390.71	390.72	364.03	364.06
		40.0	394.95	394.96	367.08	367.11
	2.1	10.0	373.37	373.38	346.71	346.74
		20.0	389.59	389.59	357.82	357.85
		30.0	397.28	397.28	362.84	362.87
		40.0	402.06	402.07	365.88	365.91

Table XI. Theoretical Performance of MMH/ClO_3F System

Chamber Pressure (psia)	Mixture Ratio	Area Ratio	I_{sp} (VAC) Equilibrium Flow: All Species	I_{sp} (VAC) Equilibrium Flow: 18 Significant Species	I_{sp} (VAC) Frozen Flow: All Species	I_{sp} (VAC) Frozen Flow: 18 Significant Species
100	1.5	10.0	306.02	306.03	294.32	294.32
		20.0	317.54	317.55	304.06	304.07
		30.0	322.99	322.99	308.52	308.51
		40.0	326.41	326.41	311.26	311.25
	1.8	10.0	311.90	311.91	293.77	293.78
		20.0	324.93	324.93	303.77	303.78
		30.0	331.10	331.11	308.35	308.36
		40.0	334.96	334.97	311.17	311.18
	2.1	10.0	313.63	313.63	290.35	290.36
		20.0	328.24	328.24	300.35	300.36
		30.0	335.25	335.25	304.95	304.96
		40.0	339.65	339.65	307.77	307.78
1000	1.5	10.0	307.02	307.03	300.92	300.94
		20.0	318.29	318.31	311.15	311.17
		30.0	323.65	323.65	315.84	315.86
		40.0	327.01	327.00	318.72	318.74
	1.8	10.0	314.18	314.19	303.09	303.12
		20.0	326.67	326.68	313.81	313.84
		30.0	332.61	332.61	318.76	318.79
		40.0	336.32	336.32	321.80	321.82
	2.1	10.0	317.63	317.63	301.18	301.22
		20.0	331.37	331.38	312.05	312.09
		30.0	337.97	337.97	317.10	317.13
		40.0	342.10	342.10	320.19	320.23

Table XII. Theoretical Performance of B_2H_6/N_2H_4 System

Chamber Pressure (psia)	Mixture Ratio	Area Ratio	I_{sp} (VAC) Equilibrium Flow All Species	Equilibrium Flow 10 Significant Species	Frozen Flow All Species	Frozen Flow 10 Significant Species
100	1.15	10.0	368.47	368.48	363.30	363.32
		20.0	385.60	385.60	379.82	379.84
		30.0	394.03	394.04	387.95	387.96
		40.0	399.43	399.43	393.14	393.15
	1.25	10.0	365.63	365.63	362.80	362.85
		20.0	382.32	382.31	379.15	379.21
		30.0	390.50	390.50	387.18	387.24
		40.0	395.74	395.73	392.31	392.37
	1.35	10.0	362.02	362.02	359.90	359.93
		20.0	378.26	378.26	375.90	375.94
		30.0	386.21	386.22	383.73	383.77
		40.0	391.28	391.28	388.72	388.76
1000	1.15	10.0	368.81	368.84	366.59	366.71
		20.0	385.87	385.89	383.39	383.52
		30.0	394.28	394.29	391.67	391.80
		40.0	399.65	399.67	396.96	397.10
	1.25	10.0	365.84	365.85	364.70	364.78
		20.0	382.48	382.48	381.21	381.29
		30.0	390.65	390.66	389.32	389.40
		40.0	395.87	395.87	394.50	394.58
	1.35	10.0	362.18	362.18	361.38	361.42
		20.0	378.39	378.39	377.50	377.54
		30.0	386.33	386.33	385.39	385.44
		40.0	391.38	391.39	390.42	390.47

Table XIII. Theoretical Performance of B_2H_6/OF_2 System

Chamber Pressure (psia)	Mixture Ratio	Area Ratio	I_{sp} (VAC) Equilibrium Flow: All Species	Equilibrium Flow: 19 Significant Species	Frozen Flow: All Species	Frozen Flow: 19 Significant Species
100	2.4	10.0	380.05	380.16	351.00	351.13
		20.0	399.82	399.91	363.42	363.54
		30.0	409.90	409.98	369.21	369.32
		40.0	416.49	416.57	372.78	372.88
	3.2	10.0	388.09	388.17	355.80	355.87
		20.0	408.71	408.78	368.17	368.24
		30.0	419.32	419.39	373.92	373.98
		40.0	426.31	426.37	377.46	377.52
	4.0	10.0	390.36	390.37	355.15	355.12
		20.0	411.28	411.29	367.31	367.26
		30.0	422.03	422.04	372.94	372.89
		40.0	429.10	429.11	376.40	376.35
1000	2.4	10.0	387.64	387.87	364.44	364.76
		20.0	407.03	407.21	378.00	378.28
		30.0	416.96	417.14	384.38	384.65
		40.0	423.54	423.71	388.33	388.60
	3.2	10.0	397.86	398.06	371.29	371.47
		20.0	418.35	418.52	384.94	385.10
		30.0	428.84	429.01	391.38	391.54
		40.0	435.75	435.90	395.38	395.52
	4.0	10.0	400.50	400.57	371.13	371.10
		20.0	421.26	421.34	384.58	384.54
		30.0	431.81	431.89	390.93	390.87
		40.0	438.70	438.76	394.86	394.79

Table XIV. Theoretical Performance of LiH/OF_2 System

Chamber Pressure (psia)	Mixture Ratio	Area Ratio	I_{sp} (VAC) Equilibrium Flow: All Species	Equilibrium Flow: 16 Significant Species	Frozen Flow: All Species	Frozen Flow: 16 Significant Species
100	2.5	10.0	346.73	346.76	322.10	322.19
		20.0	364.06	364.09	333.44	333.54
		30.0	372.91	373.93	338.72	338.82
		40.0	378.72	378.74	341.99	342.09
	3.0	10.0	352.67	352.72	322.46	322.58
		20.0	371.27	371.32	333.66	333.79
		30.0	380.68	380.72	338.86	338.99
		40.0	386.79	386.83	342.07	342.19
	3.5	10.0	351.84	351.89	320.09	320.23
		20.0	370.89	370.94	330.97	331.12
		30.0	380.66	380.70	336.00	336.15
		40.0	387.06	387.10	339.09	339.24
1000	2.5	10.0	354.00	354.04	335.21	335.35
		20.0	371.48	371.52	347.82	347.97
		30.0	380.41	380.45	353.78	353.93
		40.0	386.30	386.33	357.49	357.64
	3.0	10.0	361.04	361.10	337.48	337.65
		20.0	379.22	379.26	350.01	350.18
		30.0	388.41	388.46	355.91	356.09
		40.0	394.42	394.47	359.58	359.76
	3.5	10.0	361.02	361.09	335.49	335.67
		20.0	379.67	379.73	347.67	347.87
		30.0	389.14	389.20	353.40	353.60
		40.0	395.33	395.38	356.94	357.14

Table XV. Theoretical Performance of PBAA/Al/AP System

Chamber Pressure (psia)	Area Ratio	I_{sp} (VAC) Equilibrium Flow: All Species	I_{sp} (VAC) Equilibrium Flow: 24 Significant Species	I_{sp} (VAC) Frozen Flow: All Species	I_{sp} (VAC) Frozen Flow: 24 Significant Species
100	10.0	283.70	283.67	270.33	270.35
	20.0	299.29	299.30	282.14	282.16
	30.0	307.05	307.04	287.89	287.91
	40.0	312.03	312.03	291.52	291.55
1000	10.0	286.52	286.56	277.34	277.38
	20.0	301.70	301.71	289.74	289.78
	30.0	309.22	309.23	295.82	295.87
	40.0	314.04	314.05	299.70	299.75

Table XVI. Theoretical Performance of PBAA/Be/AP System

Chamber Pressure (psia)	Area Ratio	I_{sp} (VAC) Equilibrium Flow: All Species	I_{sp} (VAC) Equilibrium Flow: 24 Significant Species	I_{sp} (VAC) Frozen Flow: All Species	I_{sp} (VAC) Frozen Flow: 24 Significant Species
100	10.0	305.71	305.74	289.32	289.46
	20.0	324.00	324.03	303.10	303.24
	30.0	333.39	333.42	309.93	310.09
	40.0	339.56	339.58	314.32	314.48
1000	10.0	308.84	308.88	296.54	296.68
	20.0	327.15	327.18	311.01	311.16
	30.0	336.46	336.48	318.25	318.40
	40.0	342.53	342.56	322.91	323.07

Table XVII. Theoretical Performance of DB/Al/AP System

Chamber Pressure (psia)	Area Ratio	I_{sp} (VAC) Equilibrium Flow: All Species	Equilibrium Flow: 24 Significant Species	Frozen Flow: All Species	Frozen Flow: 24 Significant Species
100	10.0	284.61	284.67	272.41	272.47
	20.0	300.70	300.71	284.76	284.82
	30.0	309.26	309.20	290.86	290.93
	40.0	314.82	314.81	294.76	294.83
1000	10.0	288.46	288.54	280.52	280.65
	20.0	304.20	304.19	293.53	293.67
	30.0	312.50	312.47	300.01	300.15
	40.0	317.87	317.92	304.18	304.32

Table XVIII. Theoretical Performance of DBB/AP System

Chamber Pressure (psia)	Area Ratio	I_{sp} (VAC) Equilibrium Flow: All Species	Equilibrium Flow: 24 Significant Species	Frozen Flow: All Species	Frozen Flow: 24 Significant Species
100	10.0	303.45	303.55	289.55	289.84
	20.0	321.74	321.86	303.34	303.68
	30.0	331.19	331.25	310.20	310.37
	40.0	337.37	337.42	314.61	315.00
1000	10.0	307.31	307.40	298.09	298.27
	20.0	325.69	325.71	312.67	312.87
	30.0	335.01	335.04	320.00	320.20
	40.0	341.09	341.12	324.74	324.95

Table XIX. Chemical Reactions of Importance in Nonmetallized Propellant Systems Containing Carbon, Hydrogen, Oxygen, Nitrogen, Fluorine and Chlorine

Chemical Reaction	Chemical Reaction
$CO_2 + M \rightleftharpoons CO + O + M$	$CO + NO \rightleftharpoons CO_2 + N$
$H_2O + M \rightleftharpoons OH + H + M$	$CO + O \rightleftharpoons C + O_2$
$CO + M \rightleftharpoons C + O + M$	$HCl + Cl \rightleftharpoons H + Cl_2$
$Cl_2 + M \rightleftharpoons 2Cl + M$	$HCl + HCl \rightleftharpoons H_2 + Cl_2$
$F_2 + M \rightleftharpoons 2F + M$	$HCl + O \rightleftharpoons OH + Cl$
$HCl + M \rightleftharpoons H + Cl + M$	$HF + Cl \rightleftharpoons HCl + F$
$HF + M \rightleftharpoons H + F + M$	$HF + F \rightleftharpoons H + F_2$
$H_2 + M \rightleftharpoons 2H + M$	$HF + H \rightleftharpoons H_2 + F$
$N_2 + M \rightleftharpoons 2N + M$	$HF + HF \rightleftharpoons H_2 + F_2$
$NO + M \rightleftharpoons N + O + M$	$HF + O \rightleftharpoons OH + F$
$OH + M \rightleftharpoons O + H + M$	$HF + OH \rightleftharpoons H_2O + F$
$O_2 + M \rightleftharpoons 2O + M$	$H_2 + Cl \rightleftharpoons HCl + H$
$CO_2 + H \rightleftharpoons CO + OH$	$H_2 + O \rightleftharpoons OH + H$
$CO_2 + O \rightleftharpoons CO + O_2$	$H_2 + O_2 \rightleftharpoons 2OH$
$H_2O + Cl \rightleftharpoons OH + HCl$	$N_2 + O \rightleftharpoons NO + N$
$H_2O + H \rightleftharpoons OH + H_2$	$N_2 + O_2 \rightleftharpoons 2NO$
$H_2O + O \rightleftharpoons 2OH$	$NO + H \rightleftharpoons N + OH$
$CO + CO \rightleftharpoons CO_2 + C$	$NO + O \rightleftharpoons N + O_2$
$CO + H \rightleftharpoons C + OH$	$O_2 + H \rightleftharpoons OH + O$
$CO + N \rightleftharpoons C + NO$	

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

Chemical Reaction	Chemical Reaction
$CO + Al \rightleftharpoons AlO + C$	$O + Al_2O \rightleftharpoons 2AlO$
$CO_2 + Al \rightleftharpoons AlO + CO$	$Al_2O + M \rightleftharpoons Al + AlO + M$
$AlCl + M \rightleftharpoons Cl + Al + M$	$CO + AlCl \rightleftharpoons AlOCl + C$
$AlCl + Cl \rightleftharpoons Al + Cl_2$	$CO + AlOCl \rightleftharpoons AlCl + CO_2$
$AlCl + H \rightleftharpoons HCl + Al$	$AlCl_2 + M \rightleftharpoons Cl + AlCl + M$
$NO + Al \rightleftharpoons AlO + N$	$Cl + AlCl_2 \rightleftharpoons AlCl + Cl_2$
$AlO + M \rightleftharpoons O + Al + M$	$HCl + AlCl \rightleftharpoons AlCl_2 + H$
$O_2 + Al \rightleftharpoons AlO + O$	$NO + AlCl \rightleftharpoons AlOCl + N$
$AlO + H \rightleftharpoons Al + OH$	$AlOCl + M \rightleftharpoons O + AlCl + M$
$AlCl + O \rightleftharpoons AlO + Cl$	$O + AlOCl \rightleftharpoons AlCl + O_2$
$AlOCl + M \rightleftharpoons Cl + AlO + M$	$H + AlOCl \rightleftharpoons AlCl + OH$
$Cl + AlOCl \rightleftharpoons AlO + Cl_2$	$Cl + AlOCl \rightleftharpoons AlCl_2 + O$
$AlCl + OH \rightleftharpoons AlO + HCl$	$HCl + AlOCl \rightleftharpoons AlCl_2 + OH$
$H + AlOCl \rightleftharpoons AlO + HCl$	$2AlCl \rightleftharpoons Al + AlCl_2$
$Al + AlOCl \rightleftharpoons Cl + Al_2O$	$Al + AlOCl \rightleftharpoons AlO + AlCl$
$Cl + Al_2O \rightleftharpoons AlO + AlCl$	$Al + AlOCl \rightleftharpoons AlO + AlCl_2$
$AlCl + AlOCl \rightleftharpoons Cl_2 + Al_2O$	

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

Chemical Reactions	Chemical Reactions
$C + BeO \rightleftharpoons Be + CO$	$H + BeOH \rightleftharpoons BeO + H_2$
$CO + BeO \rightleftharpoons Be + CO_2$	$H + BeO_2H_2 \rightleftharpoons BeOH + H_2O$
$BeCl + M \rightleftharpoons Cl + Be + M$	$H_2O + BeCl \rightleftharpoons BeOH + HCl$
$Cl + BeCl \rightleftharpoons Be + Cl_2$	$O + BeOH \rightleftharpoons BeO + OH$
$H + BeOH \rightleftharpoons Be + H_2O$	$BeO_2H_2 + M \rightleftharpoons BeOH + OH + M$
$H + BeCl \rightleftharpoons Be + HCl$	$H_2O + BeO \rightleftharpoons BeOH + OH$
$N + BeO \rightleftharpoons Be + NO$	$Be_2O + H_2O \rightleftharpoons 2BeOH$
$BeO + M \rightleftharpoons Be + O + M$	$Be_2O + OH \rightleftharpoons BeO + BeOH$
$O + BeO \rightleftharpoons Be + O_2$	$Be_2O + HCl \rightleftharpoons BeCl + BeOH$
$BeOH + M \rightleftharpoons OH + Be + M$	$BeOH + M \rightleftharpoons BeO + H + M$
$H + BeO \rightleftharpoons Be + OH$	$Be_2O + Cl \rightleftharpoons BeCl + BeO$
$Be_2O + H \rightleftharpoons BeOH + Be$	$Be_2O + O \rightleftharpoons 2BeO$
$2BeOH \rightleftharpoons BeO_2H_2 + Be$	$Cl + BeO \rightleftharpoons BeCl + O$
$Be_2O + M \rightleftharpoons BeO + Be + M$	$HCl + BeCl \rightleftharpoons BeCl_2 + H$
$Cl + BeOH \rightleftharpoons BeO + HCl$	$2BeCl \rightleftharpoons BeCl_2 + Be$
$Cl + BeOH \rightleftharpoons BeCl + OH$	$BeCl_2 + M \rightleftharpoons Cl + BeCl + M$
$HCl + BeO \rightleftharpoons BeCl + OH$	$BeO + HF \rightleftharpoons F + BeOH$

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

Chemical Reaction	Chemical Reaction
$BF + M \rightleftharpoons F + B + M$	$F + BF_2 \rightleftharpoons BF + F_2$
$F + BF \rightleftharpoons B + F_2$	$HF + BF \rightleftharpoons BF_2 + H$
$BF + H \rightleftharpoons HF + B$	$BOF + M \rightleftharpoons O + BF + M$
$BN + M \rightleftharpoons B + N + M$	$BOF + H \rightleftharpoons BF + OH$
$N_2 + B \rightleftharpoons BN + N$	$BF_3 + M \rightleftharpoons F + BF_2 + M$
$BO + M \rightleftharpoons B + O$	$F + BF_3 \rightleftharpoons BF_2 + F_2$
$BO + O \rightleftharpoons O_2 + B$	$H + BF_3 \rightleftharpoons BF_2 + HF$
$BO + H \rightleftharpoons OH + B$	$BOF + F \rightleftharpoons O + BF_2$
$BF + N \rightleftharpoons F + BN$	$HF + BOF \rightleftharpoons OH + BF_2$
$N + BO \rightleftharpoons BN + O$	$2BO \rightleftharpoons BO_2 + B$
$NO + BO \rightleftharpoons BN + O_2$	$2BF \rightleftharpoons BF_2 + B$
$F + BO \rightleftharpoons BF + O$	$BF_2 + BF \rightleftharpoons B + BF_3$
$BOF + M \rightleftharpoons F + BO + M$	$BO + BF \rightleftharpoons BOF + B$
$F + BOF \rightleftharpoons BO + F_2$	$BF + BOF \rightleftharpoons BO + F_2$
$HF + BO \rightleftharpoons BF + OH$	$BO + BF_3 \rightleftharpoons BF_2 + BOF$
$H + BOF \rightleftharpoons BO + HF$	$BO + BOF \rightleftharpoons BO_2 + BF$
$HF + BO \rightleftharpoons BF + OH$	$2BOF \rightleftharpoons BO_2 + BF_2$
$BO_2 + M \rightleftharpoons O + BO + M$	$BO + C \rightleftharpoons CO + B$
$O + BO_2 \rightleftharpoons BO + O_2$	$BO + CO \rightleftharpoons CO_2 + B$
$H + BO_2 \rightleftharpoons BO + OH$	$NO + B \rightleftharpoons BO + N$
$O + BOF \rightleftharpoons BO_2 + F$	$NO + B \rightleftharpoons BN + O$
$H + BO_2 \rightleftharpoons BO + OH$	$NO + BN \rightleftharpoons BO + N_2$
$HF + BO_2 \rightleftharpoons BOF + OH$	$CO + BO \rightleftharpoons BO_2 + C$
$BO + NO \rightleftharpoons BO_2 + N$	$CO_2 + BO \rightleftharpoons BO_2 + CO$
$O + BO_2 \rightleftharpoons BO + O_2$	$CO + BF \rightleftharpoons BOF + C$
$BF_2 + M \rightleftharpoons F + BF + M$	$CO_2 + BF \rightleftharpoons BOF + CO$

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

Chemical Reaction	Chemical Reaction
$LiF + M \rightleftharpoons F + Li + M$	$H_2O + LiF \rightleftharpoons LiOH + HF$
$LiF + F \rightleftharpoons Li + F_2$	$O + LiOH \rightleftharpoons LiO + OH$
$LiH + M \rightleftharpoons H + Li + M$	$OH + LiOH \rightleftharpoons LiO + H_2O$
$H_2 + Li \rightleftharpoons LiH + H$	$O + LiF \rightleftharpoons LiO + F$
$H_2O + Li \rightleftharpoons LiH + OH$	$LiOH + M \rightleftharpoons H + LiO + M$
$H_2O + Li \rightleftharpoons LiOH + H$	$OH + LiF \rightleftharpoons LiO + HF$
$HF + Li \rightleftharpoons LiH + F$	$LiF + LiO \rightleftharpoons Li_2O + F$
$LiF + H \rightleftharpoons Li + HF$	$Li + LiOH \rightleftharpoons H + Li_2O$
$LiO + M \rightleftharpoons O + Li + M$	$H + Li_2O \rightleftharpoons LiH + LiO$
$O_2 + Li \rightleftharpoons LiO + O$	$H_2 + Li_2O \rightleftharpoons LiH + LiOH$
$OH + Li \rightleftharpoons LiH + O$	$H_2O + Li_2O \rightleftharpoons 2LiOH$
$LiOH + M \rightleftharpoons OH + Li + M$	$HF + Li_2O \rightleftharpoons LiOH + LiF$
$OH + Li \rightleftharpoons LiO + H$	$O + Li_2O \rightleftharpoons 2LiO$
$H + LiF \rightleftharpoons F + LiH$	$LiO + LiOH \rightleftharpoons Li_2O + OH$
$HF + LiF \rightleftharpoons F_2 + LiH$	$Li + LiOH \rightleftharpoons LiH + LiO$
$LiOH + H_2 \rightleftharpoons H_2O + LiH$	$Li + LiOH \rightleftharpoons Li_2O + H$
$H_2 + LiF \rightleftharpoons HF + LiH$	$Li_2O + M \rightleftharpoons Li + LiO + M$
$OH + LiO \rightleftharpoons LiH + O_2$	$Li_2O + H_2 \rightleftharpoons LiH + LiOH$
$LiOH + H \rightleftharpoons LiH + OH$	$CO + Li \rightleftharpoons LiO + C$
$H_2 + LiO \rightleftharpoons LiH + OH$	$LiO + CO \rightleftharpoons CO_2 + Li$
$HF + LiO \rightleftharpoons LiOH + F$	$LiH + Cl \rightleftharpoons HCl + Li$
$OH + LiF \rightleftharpoons LiOH + F$	$LiO + N \rightleftharpoons NO + Li$
$H + LiOH \rightleftharpoons LiO + H_2$	$LiO + HCl \rightleftharpoons Cl + LiOH$

Table XXIV. Chemical Reactions Eliminated Due to Steric Considerations

Chemical Reactions Involving No Metallized Species

$C + H_2O \rightleftharpoons CO + H_2$

$C + O_2 + M \rightleftharpoons CO_2 + M$

$CO + H_2O \rightleftharpoons CO_2 + H_2$

$H_2 + NO \rightleftharpoons H_2O + N$

$H_2 + O + M \rightleftharpoons H_2O + M$

$H_2 + O_2 \rightleftharpoons H_2O + O$

$H_2O + N \rightleftharpoons H_2 + NO$

Chemical Reactions Involving Aluminum Species

$Cl_2 + Al + M \rightleftharpoons AlCl_2 + M$

$H_2O + Al \rightleftharpoons AlO + H_2$

$Cl_2 + AlO \rightleftharpoons AlCl_2 + O$

$CO_2 + Al_2O \rightleftharpoons Al_2O_3 + C$

$Cl_2 + Al_2O \rightleftharpoons AlO + AlCl_2$

$O_2 + Al_2O + M \rightleftharpoons Al_2O_3 + M$

$H_2O + AlCl \rightleftharpoons AlOCl + H_2$

Chemical Reactions Involving Beryllium Species

$Cl_2 + Be + M \rightleftharpoons BeCl_2 + M$

$H_2O + Be \rightleftharpoons BeO + H_2$

$BeO_2H_2 + Be \rightleftharpoons Be_2O + H_2O$

$Cl_2 + BeOH \rightleftharpoons BeCl_2 + OH$

$Cl_2 + BeO \rightleftharpoons BeCl_2 + O$

$H_2O + BeO + M \rightleftharpoons BeO_2H_2 + M$

$BeCl_2 + BeO \rightleftharpoons Be_2O + Cl_2$

Chemical Reactions Involving Boron Species

$CO_2 + B \rightleftharpoons BO_2 + C$

$F_2 + B + M \rightleftharpoons BF_2 + M$

$H_2 + B + M \rightleftharpoons BH_2 + M$

$H_2O + B \rightleftharpoons BO + H_2$

$H_2O + B \rightleftharpoons BH_2 + O$

Chemical Reactions Involving Boron Species (Continued)

$O_2 + B + M \rightleftharpoons BO_2 + M$

$F_2 + BN \rightleftharpoons BF_2 + N$

$H_2 + BN \rightleftharpoons BH_2 + N$

$H_2O + BN \rightleftharpoons BH_2 + NO$

$O_2 + BN \rightleftharpoons BO_2 + N$

$F_2 + BO \rightleftharpoons BF_2 + O$

$H_2 + BO \rightleftharpoons BH_2 + O$

$H_2O + BO \rightleftharpoons BO_2 + H_2$

$H_2O + BO \rightleftharpoons BH_2 + O_2$

$F + BO_2 \rightleftharpoons BF + O_2$

$F_2 + BO_2 \rightleftharpoons BF_2 + O_2$

$H_2 + BO_2 \rightleftharpoons BO + H_2O$

$H_2 + BO_2 \rightleftharpoons BH_2 + O_2$

$N + BO_2 \rightleftharpoons BN + O_2$

$F + BH_2 \rightleftharpoons BF + H_2$

$F_2 + BH_2 \rightleftharpoons BF_2 + H_2$

$N + BH_2 \rightleftharpoons BN + H_2$

$NO + BH_2 \rightleftharpoons BN + H_2O$

$F_2 + BF + M \rightleftharpoons BF_3 + M$

$H_2O + BF \rightleftharpoons BOF + H_2$

$O + BF_3 \rightleftharpoons BOF + F_2$

Chemical Reactions Involving Lithium Species

$H_2O + Li \rightleftharpoons LiO + H_2$

$CO + LiH \rightleftharpoons LiOH + C$

$CO_2 + LiH \rightleftharpoons LiOH + CO$

$NO + LiH \rightleftharpoons LiOH + N$

$O + LiH + M \rightleftharpoons LiOH + M$

$O_2 + LiH \rightleftharpoons LiOH + O$

$C + LiOH \rightleftharpoons LiH + CO$

$F_2 + Li_2O \rightleftharpoons Li_2F_2 + O$

Table XXV. Spin Forbidden Chemical Reaction Which do no Occur in the Ground State

Chemical Reaction
$CO_2 + M \rightleftharpoons CO + O + M$
$BOF + M \rightleftharpoons O + BF + M$
$BF + BOF \rightleftharpoons BO + F_2$
$CO + AlCl \rightleftharpoons AlOCl + C$
$NO + AlCl \rightleftharpoons AlOCl + N$
$AlOCl + M \rightleftharpoons O + AlCl + M$
$C + BeO \rightleftharpoons Be + CO$
$N + BeO \rightleftharpoons Be + NO$
$BeO + M \rightleftharpoons Be + O + M$
$Be_2O + O \rightleftharpoons 2BeO$

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

Chemical Reaction	Exothermic Rate Constant	Reference
$CO_2 + M \rightleftharpoons CO + O + M$	$3 \times 10^{20} T^{-1.0} \exp -\left(\frac{11393}{T}\right)$	Avramenko, L.I. and Kolesnikova, R.V., Izvest. Akad. Navk. S.S.S.R., Otdel. Khim. Navk., 1562 (1959).
$H_2O + M \rightleftharpoons OH + H + M$	$3 \times 10^{19} T^{-1.0}$	Mayer, S.W., Cook, E.A., Schieler, L., "Nonequilibrium Recombination in Nozzles," SSD-TDR-64-139, Aerospace Corporation, Los Angeles, California, 18 Sept. 1964.
$CO + M \rightleftharpoons C + O + M$	$2 \times 10^{18} T^{-1.0}$	Wray, K.L., Avco Research Report 95 (1961).
$HF + M \rightleftharpoons H + F + M$	$1 \times 10^{19} \times 10^{-0.5}$	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.
$H_2 + M \rightleftharpoons 2H + M$	$10^{19} T^{-1.0}$	W.E. Kaskan and W.G. Browne, "Kinetics of the $H_2/CO/O_2$ System," General Electric Document No. 63SD848, 14 February 1964.
$N_2 + M \rightleftharpoons 2N + M$	$2 \times 10^{18} T^{-1.0}$	K.L. Wray, Avco Research Report 104 (1961).
$NO + M \rightleftharpoons N + O + M$	$2 \times 10^{18} T^{-1.0}$	K.L. Wray, Avco Research Report 95 (1961).
$OH + M \rightleftharpoons O + H + M$	$2 \times 10^{18} T^{-1.0}$	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.
$O_2 + M \rightleftharpoons 2O + M$	$1 \times 10^{16} T^{-0.5}$	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.
$CO_2 + H \rightleftharpoons CO + OH$	$3.2 \times 10^{12} \exp -\left(\frac{6300}{RT}\right)$	W.E. Kaskan and W.G. Browne, "Kinetics of the $H_2/CO/O_2$ System," General Electric Document No. 63SD848, 14 Feb. 1964.
$CO_2 + O \rightleftharpoons CO + O_2$	$3.58 \times 10^{15} T^{-1.0}$	L.I. Avramenko and R.V. Kilesnikova, Izvest. Akad. Navk. S.S.S.R., Otdel. Khim. Navk., 1562 (1959).
$H_2O + H \rightleftharpoons OH + H_2$	$7 \times 10^{13} \exp -\left(\frac{6100}{RT}\right)$	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.
$H_2O + O \rightleftharpoons 2OH$	$2.5 \times 10^{14} \exp -\left(\frac{10000}{RT}\right)$	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.

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

Chemical Reaction	Exothermic Rate Constant	Reference
$2CO \rightleftharpoons CO_2 + C$	$2.11 \times 10^{16} T^{-1.0}$	L.I. Avramenko, R.V. Lorentso, Zhur. Fiz. Khim., 24, 207 (1950).
$CO + H \rightleftharpoons C + OH$	$1 \times 10^{14} \exp -\left(\frac{13000}{T}\right)$	F. Kaufman and J.P. Kelso, J. Chem. Phys., 23, 1072 (1955).
$CO + N \rightleftharpoons C + NO$	$1.44 \times 10^{16} T^{-1.0}$	L.I. Avramenki and R.V. Lorentso, Zhur. FIZ. Khim., 24, 207 (1950).
$CO + NO \rightleftharpoons CO_2 + N$	$2.47 \times 10^{15} T^{-1.0}$	L.I. Avramenko and R.V. Kilesnikova, Izvest. Akad. Navk. S.S.S.R., Otdel. Khim. Navk., 1562 (1959).
$CO + O \rightleftharpoons C + O_2$	$2.48 \times 10^{13} \exp -\left(\frac{990}{T}\right)$	L.I. Avramenko and R.V. Lorentso, Zhur, Fiz, Khim., 24, 207 (1950).
$HF + H \rightleftharpoons H_2 + F$	$5 \times 10^{12} \exp -\left(\frac{5700}{RT}\right)$	S.W. Mayer, E.A. Cook, and L. Schieler, "Nonequilibrium Recombination in Nozzles," SSD-TDR-64-139, Aerospace Corporation, Los Angeles, California, 18 Sept. 1964.
$HF + O \rightleftharpoons OH + F$	$5 \times 10^{11} T^{0.5} \exp -\left(\frac{6000}{RT}\right)$	S.W. Mayer, E.A. Cook, and L. Schieler, "Nonequilibrium Recombination in Nozzles," SSD-TDR-ϕρ-139, Aerospace Corporation, Los Angeles, California, 18 Sept. 1964.
$HF + OH \rightleftharpoons H_2O + F$	$5 \times 10^{11} T^{0.5} \exp -\left(\frac{7000}{RT}\right)$	S.W. Mayer, E.A. Cook, and L. Schieler, "Nonequilibrium Recombination in Nozzles," SSD-TDR-64-139, Aerospace Corporation, Los Angeles, California, 18 Sept. 1964.
$H_2 + O \rightleftharpoons OH + H$	$1.4 \times 10^{12} \exp -\left(\frac{5190}{RT}\right)$	W.E. Kaskan and W.G. Browne, "Kinetics of the $H_2/CO/O_2$ System," General Electric Document No. 63SD848, 14 February 1964.
$H_2 + O_2 \rightleftharpoons 2OH$	$2.7 \times 10^{16} \exp -\left(\frac{53000}{T}\right)$	F. Kaufman and J.P. Kelso, J. Chem. Phys., 23, 1072 (1955).
$N_2 + O \rightleftharpoons NO + N$	$1.5 \times 10^{16} T^{-1}$	L.E. Phillips and H.I. Schiff, J. Chem. Phys., 36, 1509 (1962).
$N_2 + O_2 \rightleftharpoons 2NO$	$2.7 \times 10^{13} \exp -\left(\frac{53800}{T}\right)$	A. Ralston and H.S. Wilf, "Mathematical Method for Digital Computers," 1960.
$NO + H \rightleftharpoons N + OH$	$4.01 \times 10^{23} T^{-1}$	F. Kaufman and F.P. Del Greco, Ninth Int. Symposium on Combustion (1963).
$NO + O \rightleftharpoons N + O_2$	$1.011 \times 10^{11} T^{-0.5} \exp -\left(\frac{3120}{T}\right)$	W.G. Vincenti, Stanford Univ. Dept. Aeronaut. Engr. Rept. 101 (1961).
$O_2 + H \rightleftharpoons OH + O$	$3.2 \times 10^{11} T^{-0.47} \exp -\left(\frac{100}{RT}\right)$	W.E. Kaskan and W.G. Browne, "Kinetics of the $H_2/CO/O_2$ System," General Electric Document No. 63SD848, 14 Feb. 1964.