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THERMODYNAMICS OF COMBUSTION OF
VARIOUS PYROTECHNIC COMPOSITIONS

John E. Tanner, Jr.

Naval Ammunition Depot

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20. ABSTRACT (Continue on reverse side if necessary and identify by block number) Heats of reaction and/or adiabatic flame temperature have been computed for a variety of compositions of interest to pyrotechnics. One set of compositions includes pairwise fuel/oxidizer combinations consisting of magnesium, aluminum, beryllium, boron, carbon and silicon with alkali oxides, alkali nitrates, alkali perchlorates, teflon, air and a few other substances.		

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It has been found that the oxidizers differ from each other in approximately the same manner, regardless of which fuel is used, and similarly, the fuels differ in the same way regardless of which oxidizer is used. Significant differences in flame temperatures and heats of reaction are noted among the alkali nitrates, in spite of their similar chemistry.

Using a perchlorate as oxidizer, a large percentage of the associated alkali metal is combined as the chloride even at the adiabatic temperature.

Of six aluminum compounds tried, aluminum carbide may be competitive with magnesium metal.

Of six sodium compounds tried, the pure metal, the hydride, and the carbide are the most promising for sodium enrichment of illuminating flares.

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APPROVED BY



B. E. DOUDA, Manager
Chemical Sciences Branch
Pyrotechnic Division
Applied Sciences Department

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SUMMARY

When new or improved pyrotechnic compositions are being designed, the basic thermodynamic properties of the components and of their combustion are of immediate interest. These properties include the adiabatic flame temperature, the heat of reaction, the optimum fuel/oxidizer ratio and the concentrations and phases of product species, especially those which emit light in a wavelength range of interest. In three separate studies, flame temperature and heats of reaction have been computed for various fuel/oxidizer combinations.

The first study was a comparison of the alkali nitrates, a few oxides of sodium, hydrogen peroxide, teflon, air and oxygen as oxidizers and a comparison of aluminum, magnesium, beryllium, boron, iron, silicon and iron as fuels. About half of all the possible fuel/oxidizer pairs were formed.

It has been found that generally the oxidizers differ from each other in approximately the same manner, regardless of which fuel is used, and similarly, the fuels differ in the same way regardless of which oxidizer is used. An exception is air, whose rank among the oxidizers varies with the fuel used. Of the fuels, boron and carbon exhibit some irregularities. Significant differences in flame temperatures and heats of reaction are noted among the alkali nitrates, in spite of their similar chemistry.

Where a perchlorate was used as an oxidizer, a large percentage of the associated alkali metal was combined as the chloride even at the adiabatic temperature. This is a disadvantage for illumination purposes.

The purpose of the second study was to compare aluminum compounds as fuels for illuminating flare compositions. Of the six compounds computed, aluminum carbide has properties which may be competitive with those of magnesium. None of the compounds excelled or exceeded pure aluminum.

The purpose of the third study was to determine which sodium compounds are thermodynamically the most promising for enrichment of illuminating compositions. The most promising of six tried were found to be the pure metal, the carbide, and the hydride.

PREFACE

The Applied Sciences Department is funded to conduct exploratory studies aimed at the development of better pyrotechnic flares for signaling and illumination. The information presented here is a partial result of these efforts. A portion of these results have already been presented in RDTR No. 253, "Theoretical Light Yields From Different Illuminating Flare Compositions." See reference 1.

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INTRODUCTION

Numerous computations of flame temperatures and heats of reaction have been made for pyrotechnic compositions,^{2,3} including a few of the compositions mentioned later in this report. In order to compare a set of compositions, the computations should all be done with the same set of thermodynamic data for the reactants and products. For this reason we have repeated the computations of such well known formulations as Mg/NaNO₃/binder in order to compare with other formulations for which we could find no previous computations.

For computations of flame temperatures or of heats of reaction to products at an elevated temperature, we used the NASA computer program of Gordon and McBride.⁴

This versatile program can be used in many ways. In one option used here, a set of formulas and their heats of formation are supplied, along with the specification of the relative amounts of each and of the confining pressure. The program then computes the equilibrium temperature and mole fractions of products corresponding to adiabatic conditions.

The other option used here was to specify the final temperature. In this case, the program computes the equilibrium mole fractions of products and the final total enthalpy.

Three separate studies are presented. In the first, we compared a number of common fuels and oxidizers in simple mixtures along with a common binder. In the second study, various aluminum compounds were compared as fuels for illuminating formulations. In the third study, several sodium compounds were compared as candidates for increasing the sodium content of illuminating formulations.

FUEL/OXIDIZER PAIRS

Method

A small selection of common inorganic fuels and oxidizers has been made. Thermodynamic properties have been computed for the combustion of about half of all of the possible fuel/oxidizer combinations. For all combinations involving a solid fuel and oxidizer, five percent of epoxy binder is included, of formula C_{5.75}H_{8.36}O_{1.15}N_{0.3}.

The first step was to find for each combination the fuel/oxidizer ratio giving the highest adiabatic equilibrium temperature. The results obtained in this step also included the species mole fractions at this temperature and the theoretical density for the initial composition.

In a subsequent computation the energy of reaction was computed for reactants initially at 298K going to products at 1200K. This latter temperature was chosen as a cutoff point, below which negligible visible radiation would be given off as the reaction products cool.

The equivalence ratios were computed by dividing the weights of fuel and oxidizer by their respective gram equivalent weights, using the following valences: the fuel its maximum valence, oxygen = 2, fluorine = 1, nitrogen, chlorine, and the alkali metals = 0. The reason for assigning zero valence to nitrogen is that it usually ends almost entirely as N_2 . The alkali metals usually are in the atomic form at high flame temperatures. With the small amounts of chlorine used, the major part of it ends as a chloride of the alkali, which was already assigned zero valence. Smaller amounts do act as an oxidizer for the metal fuel and the binder. However for simplicity it was counted as inert rather than assigning to it a fractional valence, which would have been less than 0.5.

Results and Discussion

Temperatures and Heats of Reaction

The two quantities which are most important in giving an indication of the amount of energy available for visible light output are the adiabatic flame temperature (K) at equilibrium and the heat of reaction (kcal per gram of solid). These are presented together in Table 1. They correspond to the fuel/oxidizer ratios giving the maximum adiabatic temperature. Remember that the heats of reaction are for reactants at 298K going to products at 1200K.

The optimized compositions are presented in Table 2. For each composition, the first line gives the weight percent of the fuel listed in the left hand column. The next two lines give the fuel/oxidizer equivalence ratio without, and with consideration of the binder, respectively. Since the binder is a fuel (the equivalent weight of epoxy binder is 3.44) the second number is always larger than the first.

In comparing the alkali nitrates, the small differences in adiabatic temperature are much magnified in the heats of reaction. This is partially due to the varying amounts of alkali metal oxidized at the cutoff temperature of 1200K (data not presented). A computation with products at 298K would show the various alkali nitrates to have more nearly equal heats of reaction.

In the case of silicon, comparing sodium nitrate with sodium perchlorate, a small difference in adiabatic temperature corresponds to a large difference in heat of reaction. Again it is a matter of the degree of reaction of the sodium at the cutoff point of 1200^oK. At this temperature the perchlorate sodium is completely combined as chloride, whereas the nitrate sodium is mostly in elemental form, and will liberate a large amount of energy when it reacts with the water and other oxides present as the temperature is lowered toward 298K.

The high heats of reaction obtained with air or oxygen as the oxidizer are not the result of any unusual chemistry, but simply result from not including them in the calculation of the total weight of reactants. This was done because in actual usage these gases are in the environment and thus may be had "free".

Optimum Fuel/Oxidizer Ratios

Generally it can be expected that a stoichiometric mixture yields the highest temperature. However, several factors can cause this expectation not to be precisely fulfilled:

The most common deviation here is caused by the competition between two fuels of greatly different reducing powers--a metal and a binder. An optimum is reached when the weaker fuel is only partly oxidized. Hence in nearly all cases in Table 2, the optimum equivalence ratio counting the binder, and that not counting the binder lie on opposite sides of unity. The closer the latter is to unity, the more successful the metal is in excluding the binder from the available oxygen.

When the product of combustion is considerably dissociated at equilibrium, the optimum is shifted in the direction of the component having the lowest heat capacity

and/or the most positive heat of formation. This is well demonstrated in the mixtures with air, where the optimum fuel/oxidizer ratios are relatively high.

The low equivalence ratios seen in the combinations of carbon and iron with sodium nitrate can be explained by the low flame temperatures in these cases. The sodium is able to compete for the oxygen and so should have been included as a fuel in calculating the fuel/oxidizer equivalence ratio.

Reaction Products

There is a wealth of information in the listings of reaction products in Table 3. Only a few things will be pointed out:

For all but the weakest fuels, carbon and iron, the alkali elements are present mostly in the atomic form when chlorine is absent. Except for the case of lithium, the atomic form accounts for more than 95% of the total.

When perchlorate is the oxidizer, however, a large portion of the alkali elements are present in the form of the chloride. Other calculations (not presented) show that the percentage of chloride increases rapidly as the mixture cools below the adiabatic temperature.

The metals vary considerably in the extent of dissociation of the oxidation product at equilibrium. Magnesium oxide or chloride is the least stable, with increasing stability for the compounds of aluminum, beryllium, boron, and iron, in that order.

Boron nitride is sufficiently stable so that nitrogen can be an effective oxidizer of boron after all the oxygen has been consumed, and can influence the optimum composition. An example is seen in the case of boron plus air.

Table 4 gives computed densities of various fuel-oxidizer combinations.

Example of a Prediction

The purpose of accumulating this data has been to help in predicting luminous output. As an example, we might use the numbers in Tables 1 and 2 to predict relative output of the sodium-containing oxidizers used with magnesium as fuel.

The heats of reaction and adiabatic temperatures both indicate that light output when using sodium peroxide (Na_2O_2) should be much lower than for the other cases. This has been verified by experiment.

Sodium superoxide should have a slight edge over sodium nitrate due to a somewhat higher heat of reaction and a significantly higher sodium atom content.

A comparison between sodium perchlorate and sodium nitrate is more difficult. The thermodynamic factors both favor the sodium perchlorate, but the tying up of the perchlorate sodium by the chlorine operates in favor of the nitrate as yielding the greater light output. A computation where these factors are combined in a more sophisticated manner might be able to successfully predict the result.

ALUMINUM COMPOUNDS

Introduction

Aluminum has for some time been considered a very promising compound for illumination pyrotechnics because of the high flame temperatures which it is theoretically capable of attaining in combustion. Test results have not borne out these expectations. The failure is believed due to incompleteness of combustion of the aluminum, which is in turn caused by the very low volatility of the metal and its oxide.

One way of more completely exposing all of the aluminum to the oxidizer would be to have it present in the form of a molecular compound, with the other elements being more volatile. A penalty would be paid for the presence of these elements, since they would almost certainly have lower energies of combustion, and thus would lower the reaction temperature.

We have here investigated which aluminum compounds would be most promising by computing adiabatic flame temperatures of various ones, in each case reacting with a stoichiometric amount of sodium nitrate. No binder is included. Where carbon or sulfur is involved and the stoichiometry is in doubt, several fuel/oxidizer ratios were calculated and the maximum temperature estimated.

Results and Discussion

The computed flame temperatures of the aluminum compounds and of magnesium are presented in Table 5. As expected, all of the calculated adiabatic temperatures fall below that for metallic aluminum. Furthermore only one compound, aluminum carbide, gives an adiabatic temperature above that for magnesium metal, which is the present standard pyrotechnic fuel.

It is doubtful that aluminum carbide is promising even from a thermodynamic standpoint in comparison to magnesium for illumination pyrotechnics. Although the former has a higher theoretical flame temperature, this would be at least partially offset by its lower heat of combustion.

ENRICHMENT WITH SODIUM COMPOUNDS

Introduction

It is well known that the principal emitter in illumination formulations is the sodium atom. The possibility exists then that an increase in the sodium content of the composition might increase the light emission.

The final result will be determined by several conflicting factors. One of these is that sodium compounds are not very energetic in the flare reactions, and thus their presence will decrease the flame temperature.

To determine which sodium compounds would be most promising for increasing the sodium content, we have computed flame temperatures for a basic mixture of 3 moles magnesium and 1 mole sodium nitrate, to which an additional mole of sodium-containing compound is added. This additional mole is balanced between the compound under consideration and a stoichiometric amount of sodium nitrate. Thus the proportions when adding sodium amide are: $3 \text{ Mg} + 1.25 \text{ NaNO}_3 + .75 \text{ NaNH}_2$. In computing stoichiometry, several valences were tried for carbon and sulfur. Those giving the maximum temperatures were 3 and 4, respectively.

Results and Discussion

The compositions and computed adiabatic flame temperatures are presented in Table 6. It can be seen that, judging by computed flame temperature, the best method of increasing sodium content is by the addition of metallic sodium itself. Next best would be the addition of the hydride or carbide.

Although heats of reaction have not been computed for these formulations, it seems probable that they lie in about the same order as the flame temperatures.

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TABLE 1

Computed adiabatic temperatures (K) and heats of reaction (kcal/g, products at 1200K) of fuel-oxidizer combinations. 5% epoxy binder is included where both fuel and oxidizer are solids.

	LiNO ₃	NaNO ₃	KNO ₃	CsNO ₃	NaClO ₄	KClO ₄	NaO ₂	Na ₂ O ₂	H ₂ O ₂	-CF ₂ -	Air	O ₂
Al	3361 2.15	3371 1.47	3326 1.20	3146 .64	3594 2.32	3580 2.08	3460 1.65	2260 .49	3440 3.00	3460	3549 5.97	4019 6.95
Mg	3084 1.93	3073 1.45	3056 1.17	2970 .63	3156 2.08	3154 1.89	3089 1.64	2339 .56	3150 2.70	3400 1.93	3053 3.66	3347 5.48
Be		3554 1.98			3736 2.97					3607	3538 12.9	
B		2151 1.16			3151 2.03					3518 1.20	2728 7.1	
Fe		1775 2.81			2727							
Si		2855 1.10			2998 1.93						2846 5.6	
C		1640 .33			2756 .93						2236 4.4	

TABLE 2

Weight percent fuel and fuel/oxidizer equivalence ratios to produce the maximum computed adiabatic temperature.

	LiNO ₃	NaNO ₃	KNO ₃	CsNO ₃	NaClO ₄	KClO ₄	NaO ₂	Na ₂ O ₂	H ₂ O ₂	Air	O ₂
Al	38.7 ^a	34.4	30.3	17.1	34.5	31.3	35.2	27.2	50.3	20.6	52.4
	.87 ^b	.90	.88	.79	.97	.94	.90	.87	.95	1.07	.98
	1.17 ^c	1.24	1.25	1.40	1.34	1.34	1.23	1.28			
Mg	43.0	39.9	35.2	20.2	38.1	35.1	40.8	33.0	53.5	29.0	60.2
	.78	.85	.82	.72	.85		.85	.85	.80	1.24	1.00
	1.10	1.22	1.23	1.36	1.24		1.22	1.31			
Be	21.3				20.6					11.2	
	.91				.94					1.04	
	1.19				1.24						
B	17.6				15.7					22.2	
	.89				.84					2.92	
	1.16				1.12						
Fe	39.				49.						
	.53				.89						
	.90				1.37						
Si	26.8				26.4					17.5	
	.80				.84					1.12	
	1.10				1.17						
C	10.6				14.2					7.8	
	.60				.90					1.05	
	.84				1.17						

- a - Weight percent fuel
- b - F/O equivalence ratio not counting binder
- c - F/O equivalence ratio counting binder

TABLE 3
MOLE FRACTIONS OF REACTION PRODUCTS
(A) ALUMINUM FUEL

LiNO ₃		NaNO ₃		KNO ₃		CSNO ₃		NaClO ₄	
AL	.00576	AL	.00802	AL	.00590	AL	.00204	AL	.02525
ALH	.00003	ALH	.00005	ALH	.00004	ALH	.00003	ALCL	.03110
ALO	.00224	ALO	.00268	ALO	.00174	ALO	.00053	ALCL-	.06130
ALOH	.00052	ALOH	.00069	ALOH	.00064	ALOH	.00057	ALH	.00004
ALOH+	.06199	ALOH+	.07261	ALOH+	.06664	ALOH+	.04324	ALO	.01122
ALO2	.00062	ALOH-	.00001	ALOH-	.00001	ALOH-	.00001	ALOCI	.00887
ALO2-	.02891	ALO2	.00064	ALO2	.00046	ALO2	.00010	ALOH	.00654
ALO2H	.00054	ALO2-	.03285	ALO2-	.02871	ALO2-	.01383	ALOH+	.13448
AL2O	.00123	ALO2H	.00062	ALO2H	.00061	ALO2-	.00043	ALO2	.03445
AL2O-	.00001	AL2O	.00168	AL2O	.00130	AL2O	.00034	ALO2-	.14245
AL2O-(L)	.21810	AL2O-	.00002	AL2O-	.00001	AL2O-(L)	.17604	ALO2H	.00002
CO	.10362	AL2O-(L)	.19820	AL2O-(L)	.19665	CO	.18175	AL2O	.00002
CO2	.00454	CO	.11243	CO	.12383	CO2	.00542	AL2O-	.00004
CO2-	.00003	CO2	.04425	CO2	.00460	CO2-	.00005	AL2O-(L)	.14314
E	.03274	CO2-	.00004	CO2-	.00004	CS	.25444	CO	.12000
H	.03952	E	.03943	E	.03900	CS+	.00093	CO2	.10572
H-	.00003	H	.04792	H	.05134	CSO	.00053	CO2-	.00003
H2	.01116	H-	.00004	H-	.00004	CS2	.00011	CL	.04477
H2O	.00385	H2	.01520	H2	.02224	E	.03012	CL-	.06590
LI	.28068	H2O	.00444	H2O	.00644	H	.05674	CLO	.00000
LI+	.00001	N	.00004	K	.28107	H-	.00005	E	.02900
LIH	.00092	NO	.00256	K+	.00033	HCO	.00001	H	.02870
LIN	.00001	NO2-	.00001	KO	.00144	H2	.06714	H-	.00001
LIO	.00412	N2	.14655	KOH	.00266	H2O	.01605	HCL	.00430
LIO-	.00002	NA	.28619	K2	.00004	N	.00001	H2	.06130
LIOH	.01780	NA+	.00003	N	.00003	NO	.00004	H2O	.00071
LI2	.00018	NAH	.00046	NO	.00213	N2	.13572	N	.00002
LI2O	.00211	NAO	.00106	NO2-	.00001	O	.00261	NO	.00101
N	.00004	NAO-	.00004	N2	.14531	O-	.00004	N2	.00270
NO	.00292	NAOH	.00166	O	.00889	OH	.00500	NA	.15500
NO2-	.00001	NA2	.00004	O-	.00011	OH-	.00011	NA+	.00001
N2	.15541	O	.01153	OH	.00641	O2	.00025	NaCL	.00960
O	.01240	O-	.00014	OH-	.00011			NAH	.00000
O-	.00013	OH	.00617	O2	.00164			NAO	.00120
OH	.00590	OH-	.00010					NAO-	.00000
OH+	.00008	O2	.00136					NAOH	.00000
O2	.00171							NA2	.00000
								O	.00000
								O-	.00000
								OH	.00000
								OH-	.00000
								O2	.00000

TABLE 3 (CONT.)

(A) ALUMINUM FUEL (CONT.)

KClO ₄		NAO ₂		NA ₂ O ₂		H ₂ O ₂		-CF ₂ -	
AL	.02353	AL	.01043	AL	.00002	AL	.01214	ALF	.0177
ALCL	.02322	ALH	.00005	ALOH	.00001	ALH	.00022	ALF2	.03775
ALCL-	.00077	ALO	.00371	ALOH+	.00067	ALO	.00451	ALF3	.26950
ALH	.00005	ALOH	.00070	AL2O3(S)	.18299	ALOH	.00311	C(S)	.44500
ALO	.01036	ALOH+	.08062	CO	.10400	ALOH+	.18339	C	.00000
ALDCL	.00660	ALOH-	.00001	CO2	.00010	ALOH-	.00006	CF	.02370
ALOH	.00066	ALO2	.00094	E	.00007	ALOH-	.00018	CF2	.00000
ALOH+	.14229	ALO2-	.03894	H	.00191	ALU2	.09079	CF3	.00000
ALO2	.00315	ALO2H	.00006	H2	.07339	ALO2-	.03002	CF4	.00000
ALO2-	.04769	AL2O	.00252	H2O	.00037	ALO2H	.00296	CN	.00027
ALO2H	.00073	AL2O2	.00002	N2	.00273	AL2O	.00003	C2	.00000
AL2O	.00629	AL2O3(L)	.18772	NA	.02854	AL2O2	.00003	C2F2	.00000
AL2O-	.00007	CO	.10940	NAH	.00101	AL2O3(L)	.12690	C2N	.00017
AL2O3(L)	.14068	CO2	.00434	NAOH	.00051	E	.09091	C2N2	.00000
CO	.13098	CO2-	.00004	NA2	.00187	H	.19859	C3	.00000
CO2	.00616	E	.04132			H-	.00029	C4	.00000
CO2-	.00003	H	.04572			H2	.17269	C5	.00000
CL	.03367	H-	.00003			H2O	.05619	F	.07765
CL-	.06037	H2	.01043			U	.01990	FCN	.00135
CLO	.00002	H2O	.00334			U-	.00042	N	.00000
F	.03444	N	.00001			UH	.12937	N2	.11478
H	.03582	NO	.00044			UH-	.00002		
H-	.00002	N2	.00274			U2	.00258		
HCL	.00428	NA	.42585						
H2	.00304	NA+	.00095						
H2O	.00115	NAH	.00057						
K	.12676	NAO	.00187						
K+	.00061	NAO-	.00006						
KCL	.09005	NAOH	.00211						
RO	.00186	NA2	.00019						
KOH	.00045	O	.01691						
K2	.00031	O-	.00017						
N	.00002	UH	.00643						
NO	.00101	UH-	.00009						
N2	.00307	U2	.00200						
O	.04638								
O-	.00028								
OH	.00670								
OH-	.00005								
O2	.00645								

AIR		O ₂	
AL	.03271	AL	.17857
AL+	.00013	AL+	.00139
ALO	.01042	ALO	.10052
ALU2	.00230	ALO2	.03717
ALU2-	.00007	ALU2-	.00105
AL2O	.00991	AL2O	.06620
AL2O2	.00004	AL2O+	.00004
AL2O3(L)	.10498	AL2O2	.00043
E	.00000	AL2O3(L)	.21118
N	.00023	E	.00037
NO	.01087	U	.34016
N2	.79492	U-	.00001
O	.03002	U2	.06237
O2	.00329		

TABLE 3 (CONT.)
(B) MAGNESIUM FUEL

LiNO ₃		NaNO ₃		KNO ₃		CSNO ₃		NaClO ₄		KClO ₄	
CO	.06558	CO	.06986	CO	.07747	CO	.1977	CO	.07697	CO	.08410
CO2	.01967	CO2	.01981	CO2	.02140	CO2	.02734	CO2	.02604	CO2	.02680
E	.00015	E	.00027	CO2-	.00001	CO2-	.00003	CL	.02031	CL =	.01458
H	.01087	H	.01753	E	.00115	CS	.19226	CL-	.00063	CL-	.00187
H2	.00468	H2	.01266	H	.01791	CS+	.00257	CLO	.00003	CLO	.00002
H2O	.01032	H2O	.02634	H2	.01455	CSO	.00156	E	.00007	F	.00028
LI	.13264	MG	.08254	H2O	.02936	CS2	.00002	H	.02119	H	.02308
LI+	.00015	MGH	.00029	K	.18378	CS2O	.00001	HCL	.01502	HCL	.01189
LIH	.00034	MGN	.00001	K+	.00119	E	.00247	H2	.01067	H2	.01282
LI0	.00716	MGO(S)	.36403	KO	.00446	H	.02103	H2O	.02702	H2O	.03055
LI0H	.00721	MGO	.05507	KOH	.01412	H2	.03227	MG	.11067	K	.04183
LI2	.00007	MGOH	.01031	K2	.00005	H2O	.05265	MGCL	.01064	K+	.00213
LI2O	.00008	MGO2H2	.00030	MG	.07728	MG	.05958	MGCL2	.01101	KCL	.11808
LI2O2	.00005	N	.00001	MGH	.00029	MGH	.00031	MGH	.00035	KO	.00154
MG	.08097	NO	.00406	MGN	.00001	MGN	.00001	MGO(L)	.31625	KOH	.00312
MGN	.03017	N2	.10146	MGO(S)	.36118	MGO(S)	.32891	MGO	.10027	MG	.11648
MGN	.00001	NA	.18902	MGO	.04886	MGO	.02699	MGOH	.01323	MGCL	.00810
MGO(S)	.37888	NA+	.00028	MGOH	.01028	MGOH	.01063	MGO2H2	.00037	MGCL2	.00609
MGO	.05814	NAH	.00029	MGO2H2	.00031	MGO2H2	.00042	NO	.00107	MGH	.00040
MGOH	.00650	NAO	.00223	N	.00001	NO	.00205	N2	.00215	MGO(L)	.31394
MGO2H2	.00012	NAOH	.01035	NO	.00368	NO2-	.00001	NA	.06325	MGO	.09898
N	.00001	NA2	.00007	NO2-	.00001	N2	.10104	NA+	.00070	MGOH	.01440
NO	.00469	O	.01098	N2	.10255	O	.00454	NaCl	.09784	MGO2H2	.00042
N2	.11183	OH	.01299	O	.00956	O-	.00001	NAH	.00004	NO	.00104
O	.01221	O2	.00922	O-	.00001	OH	.01128	NAO	.00115	N2	.00237
OH	.00861			OH	.01270	OH-	.00004	NAOH	.00345	O	.02263
O2	.01087			OH-	.00002	O2	.00351	NA2	.00001	OH	.02077
				O2-	.00779			NA2CL2	.00001	OH-	.00001
								O	.02439	O2	.02170
								OH	.02030		
								O2	.02483		

NaO ₂		Na ₂ O ₂		H ₂ O ₂	
CO	.06852	CO	.08216	E	.00001
CO2	.01978	CO2	.00112	H	.06312
E	.00036	E	.00001	HO2	.00001
H	.01758	H	.00212	H2	.09400
H2	.01133	H2	.05246	H2O	.18593
H2O	.02408	H2O	.00370	MG	.14356
MG	.09070	MG	.00747	MG+	.00001
MGH	.00030	MGH	.00004	MGH	.00131
MGO(S)	.35046	MGO(S)	.38600	MGO(L)	.28792
MGO	.06323	MGO	.00005	MGO	.10084
MGOH	.01059	MGOH	.00029	MGOH	.03932
MGO2H2	.00029	N2	.00218	MGO2H2	.00255
NO	.00063	NA	.45443	U	.01913
N2	.00199	NA+	.00001	OH	.04705
NA	.28385	NAH	.00118	O2	.01522
NA+	.00037	NAO	.00001		
NAH	.00041	NAOH	.00442		
NAO	.00354	NA2	.00112		
NAOH	.01464	OH	.00003		
NA2	.00015				
O	.01275				
OH	.01348				
OH-	.00001				
	.01093				

-CF ₂ -	AIR	O ₂			
C(S)	.45316	MG	.10593	E	.00002
C	.0170	MGN	.00003	MG	.23624
CF	.07	MGO(S)	.20054	MG+	.00002
CF2	.02	MGO	.06007	MGO(L)	.32379
CH	.0224	N	.00001	MGO	.28228
Cl	.0000	NO	.00492	O	.07608
Cl2	.0110	N2	.06611	O2	.08109
Cl2	.00004	O	.01060		
Cl3	.00405	O2	.00778		
C4	.00002				
C5	.0000				
F	.3197				
FCO	.0017				
MG	.00002				
MGH	.3004				
MGO	.44745				
N	.00001				
N2	.111				

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**TABLE 3 (CONT.)
(C) BERYLLIUM FUEL**

NANO ₃		NACLO ₄		-CF ₂ -		AIR	
BE	.02246	BE	.04991	BE	.00047	BE	.03150
BEH	.00012	BECL	.01479	BEF	.05564	BEH	.00004
BEN	.00001	BECL ₂	.01031	BEF ₂	.47059	BE(OH) ₂	.05309
BE(OH) ₂	.48916	BEH	.00019	C(S)	.41065	BE(OH) ₃	.00378
BE(OH) ₃	.00284	BE(OH) ₃ (L)	.42969	C	.00386	BE ₂ O	.00739
BEOM	.00506	BE(OH) ₃ (L)	.00852	CF	.00842	BE ₂ O ₂	.00447
BE(OH) ₂	.00028	BEOM	.00589	CF ₂	.00922	BE ₃ O ₃	.00555
BE ₂ O	.00538	BE(OH) ₂	.00023	C ₂	.00367	BE ₄ O ₄	.00282
BE ₂ O ₂	.00333	BE ₂ O	.01375	C ₃	.02649	N	.00019
BE ₃ O ₃	.00804	BE ₂ O ₂	.00919	C ₄	.00017	NO	.00644
BE ₄ O ₄	.00146	BE ₃ O ₃	.00870	C ₅	.00038	N ₂	.66693
CO	.06565	BE ₄ O ₄	.00303	F	.01944	O	.01749
CO ₂	.00172	CO	.07363			O ₂	.00140
E	.00113	CO ₂	.00235				
H	.05440	CL	.06224				
H ₂	.01322	CL-	.00197				
H ₂ O	.00279	CLO	.00004				
N	.00006	CL ₂	.00001				
NO	.00228	E	.00073				
N ₂	.10226	H	.06391				
NA	.20007	HCL	.01122				
NA+	.00114	H ₂	.00763				
NAH	.00038	H ₂ O	.00201				
NAO	.00080	N	.00002				
NAOH	.00084	NO	.00067				
NA ₂	.00006	N ₂	.00163				
O	.01335	NA	.10686				
OH	.00556	NA+	.00271				
O ₂	.00112	NACL	.04994				
		NAH	.00015				
		NAO	.00078				
		NAOH	.00035				
		NA ₂	.00001				
		O	.04338				
		O-	.00001				
		OH	.00899				
		O ₂	.00452				

(D) BORON FUEL

NACLO ₄		NANO ₃		-CF ₂ -		AIR	
BCL	.00003	B	.00331	H	.00001	B(L)	.02097
BO	.09121	B ₂ O	.00017	BF	.03414	b	.00113
BOCL	.00985	B ₂ O ₂	.00014	BF ₂	.05200	BN(S)	.26199
B ₂ O	.08041	B ₂ O ₂	.00094	BF ₃	.31903	BN	.00014
B ₂ O ₂	.00298	B ₂ O ₃ (L)	.05037	C(S)	.52079	BO	.13511
B ₂ O ₃	.00293	B ₂ O ₃	.213.2	C	.00172	B ₂ O	.00004
B ₂ O ₃	.18113	CO	.10619	CF	.01594	B ₂ O ₂	.00002
CO	.11132	CO ₂	.00081	CF ₂	.00172	B ₂ O ₂	.00740
CO ₂	.01329	H	.00088	CL	.00149	B ₂ O ₃	.00272
CL	.04595	HBO	.00003	C ₃	.01133	N ₂	.49461
CL-	.00037	HBO ₂	.05708	C ₄	.00006		
CLO	.00003	H ₂	.04542	C ₅	.00014		
CL ₂	.00001	H ₂ O	.00174	F	.04160		
E	.00003	N ₂	.17242				
H	.12530	NA	.33551				
HBO	.00009	NA+	.00014				
HBO ₂	.07638	NAH	.00008				
HCL	.02860	NAOH	.00187				
H ₂	.01078	NA ₂	.00007				
H ₂ O	.00951						
NO	.00052						
N ₂	.00299						
NA	.07967						
NA+	.00337						
NACL	.19608						
NAH	.00004						
NAO	.00050						
NAOH	.00128						
NA ₂	.00001						
NA ₂ CL ₂	.00003						
O	.01214						
OH	.00853						
O ₂	.0436						

TABLE 3 (CONT.)

(E) IRON FUEL

(F) SILICON FUEL

NANO ₃		NACLO ₄	
CO	.00035	CO	.06781
CO ₂	.19664	CO ₂	.09013
FE _{3O₄} (S)	.16284	CL	.00582
H ₂	.00001	CLO	.00001
H ₂ O	.01077	FE	.00356
NO	.00036	FECL	.00011
N ₂	.22854	FECL ₂	.00269
NA	.07983	FE ₂ O(L)	.47530
NAO	.00135	FE ₂ O	.00233
NAOH	.26280	FE ₂ O ₂ H ₂	.00034
NA ₂	.00018	H	.00445
NA ₂ O(L)	.05044	HCL	.01829
NA ₂ O ₂ H ₂	.00099	H ₂	.00979
O	.00001	H ₂ O	.00551
OH	.00007	NO	.00505
O ₂	.00564	N ₂	.00384
		NA	.02388
		NA ₂ CL	.17505
		NAH	.00003
		NAO	.00039
		NAOH	.00531
		NA ₂ CL ₂	.00014
		O	.00305
		OH	.01029
		O ₂	.01103

NANO ₃		NACLO ₄		AIR	
CO	.05881	CO	.06509	NO	.01191
CO ₂	.04700	CO ₂	.05618	N ₂	.75496
E	.00014	CL	.02827	O	.00835
H	.00741	CL-	.00056	O ₂	.01863
H ₂	.00706	CLO	.00007	SiO	.10133
H ₂ O	.04237	CL ₂	.00001	SiO ₂ (L)	.09933
NO	.00595	E	.00003	SiO ₂	.00548
NO ₂ -	.00021	H	.01255		
N ₂	.14794	HCL	.02444		
NA	.25677	H ₂ O	.00001		
NA+	.00016	H ₂	.00746		
NAH	.00027	H ₂ O	.04639		
NAO	.00404	NO	.00155		
NAOH	.03386	N ₂	.00239		
NA ₂	.00614	NA	.04607		
O	.00741	NA+	.00059		
OH	.01223	NACL	.18315		
O ₂	.01071	NAH	.00005		
SiO	.08778	NAO	.00130		
SiO ₂ (L)	.25936	NAOH	.00535		
SiO ₂	.00484	NA ₂ CL ₂	.00004		
		O	.02715		
		OH	.02622		
		O ₂	.06834		
		SiO	.04496		
		SiO ₂ (L)	.13462		
		SiO ₂	.01713		

(G) CARBON FUEL

NANO ₃		NACLO ₄		AIR	
CO	.00037	CO	.23958	CO	.02530
CO ₂	.48580	CO ₂	.34170	CO ₂	.17619
H ₂ O	.00164	CL	.01412	NO	.00166
NO	.00011	CL-	.00025	N ₂	.79398
N ₂	.20814	CLO	.00002	O	.00018
NA	.02491	CL ₂	.00001	O ₂	.00278
NAO	.00024	E	.00001		
NAOH	.16936	H	.00523		
NA ₂	.00001	HCL	.02177		
NA ₂ O(L)	.10782	H ₂	.00564		
OH	.00001	H ₂ O	.05393		
O ₂	.00157	NO	.00080		
		N ₂	.00257		
		NA	.02970		
		NA+	.00020		
		NACL	.22502		
		NAH	.00002		
		NAO	.00058		
		NAOH	.00561		
		NA ₂ CL ₂	.00011		
		O	.00802		
		OH	.01363		
		O ₂	.03143		

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AL	.00047
AL ₂ O	.00008
AL ₂ O ₃	.00007
AL ₂ O ₃ (L)	.31295
FE(L)	.54631
FE	.07952
FE ₂ O	.00075
NO	.00005
N ₂	.05471
O	.00017

TABLE 4

Computed Densities (g/cc) of Fuel-Oxidizer Combinations.

	LiNO ₃	NaNO ₃	KNO ₃	CsNO ₃	KClO ₄	Na ₂ O ₂	H ₂ O ₂	-CF ₂ -
Al	2.28	2.20	2.09	3.00	2.34	2.49	1.88	2.32
Mg	1.91	1.88	1.84	2.65	2.01	2.13	1.59	2.02
Be		1.97						2.11
B		2.11						2.23
Fe		2.81						
Si		2.12						
C		2.09						

TABLE 5

Computed adiabatic temperatures for the combustion of aluminum compounds.

Reaction	Temperature (K)
$2\text{Al} + \text{NaNO}_3$	3758
$\text{Al}_4\text{C}_3 + 3 \text{NaNO}_3$	3321
$3 \text{Mg} + \text{NaNO}_3$	3158
$6 \text{Mg}_4\text{Al}_3 + 17 \text{NaNO}_3$	3147
* $\text{AlH}_3 + \text{NaNO}_3$	2879
* $3 \text{MgAl}_2\text{H}_8 + 8 \text{NaNO}_3$	2794
* $6 \text{LiAlH}_4 + 7 \text{NaNO}_3$	2448
$\text{Al}_2\text{S}_3 + 3 \text{NaNO}_3$	1616

* A considerably higher adiabatic temperature would probably be computed for a more fuel-rich mixture.

TABLE 6

Computed adiabatic temperature for enrichment with sodium compounds.

Fuel Compound Added	Temperature (K)
No additive	3158
Na	3098
Na_2C_2	3048
NaH	3046
Na_2S	3017
NaN_3	3010
NaNH_2	2987