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Research paper

Computational Determination of the Specific Impulse of Solid Rocket Propellant Compositions of *closo*-Dodecaborate ($[B_{12}H_{12}]^{2-}$) Salts with HTPB Binder and Ammonium Perchlorate as an Oxidizer

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Abstract: Boron (B) powder in elemental form is a very attractive high-energy material and it is a metalloid chemical element. B powder has the second highest heat of explosion of any element that can be adopted as an energetic material in dealing with propellants and explosives. In practical situations, B has problems with ignition and combustion due to the formation of a B_2O_3 layer on its surface. B cannot burn easily; it requires ultra-pure oxygen during the combustion process and also undergoes agglomeration due to which incomplete combustion of the B particles in the propellant composition occurs. Hence in order to address these issues, we introduced *closo*-dodecaborate ($[B_{12}H_{12}]^{2-}$) salts into a solid rocket propellant composition instead of B powder. In the present work, three solid rocket propellant compositions based on *closo*-dodecaborate salts were theoretically investigated. The specific impulse (I_{sp}) was calculated for three *closo*-dodecaborate-$[B_{12}H_{12}]^{2-}$ based propellant compositions using the EXPLO5 code version V6.03. The performance values of the *closo*-dodecaborate $[B_{12}H_{12}]^{2-}$ salts based propellant compositions were compared with those of pure aluminium (Al)-based composite propellant. Using the EXPLO5 code (V6.03); hydroxyl-terminated polybutadiene (HTPB) and ammonium perchlorate (NH_4ClO_4, AP) were used as binder and oxidizer respectively. *closo*-Dodecaborate salts-HTPB-AP formulations have good theoretical performance; it was observed that the presence of a *closo*-dodecaborate salt in the propellant composition can lead to very good performance, and they are potential candidates as fuels and/or fuel additives in propellant compositions for missile and rocket applications.

Keywords: *closo*-dodecaborate salts, 3,3′-(but-2-yne-1,4-diyl)*bis*(1-methyl-1*H*-imidazol-3-ium)dodecaborate, *bis*(triethylammonium)dodecaborate, *bis*(butylmethylimidazolium)dodecahydroborate, EXPLO5, specific impulse

Symbols and Abbreviations:

BAM-H1 3,3′-(But-2-yne-1,4-diyl) *bis*(1-methyl-1*H*-imidazol-3-ium)dodecaborate
BAM-H2 *bis*(Triethylammonium)dodecaborate
BAM-H3 *bis*(Butylmethylimidazolium)dodecahydroborate

Supplementary Information: Supplementary information (SI) contains the original calculations of the I_{sp} values of different propellant compositions through EXPLO5 version 6.03.

1 Introduction

A ramjet with solid rocket propellant is a smart idea as it successfully uses atmospheric air during its action. It has great advantages in terms of increasing the variety of a missile's payload capacity. Fuel-rich solid-fuel rocket propellants are designed, equipped, and projected for ramjets. Using high specific impulse (I_{sp}), fuel-rich solid rocket propellants can still produce high thrust even though a small nozzle throat area. Frequently used fuels are listed in Table 1. Propellants containing highly energetic materials can give high I_{sp} values [1-4]. Boron (B) is a likely component of rocket propellants, used in fuel-rich propellants. It is better than beryllium (Be), magnesium (Mg) and Al *etc*. because its oxides (esp. BeO) are very toxic. B-based fuel-rich rocket solids are a type of composite solid propellant with binders as a matrix and solid fillers. Their main components are macromolecular binders (*e.g.* HTPB), oxidizers (*e.g.* AP), metallic fuels (*e.g.* B, Mg or Al powders), ballistic modifiers, plasticizers, and curing agents, used to impart specific performance to the fuel-rich propellant. Additives with various functions and performance modifiers are also added to the fuel formulation, such as combustion catalysts, binders and antioxidants.

In recent years, an important development method is to add metallic components to advanced solid rocket propellant compositions. B, Mg and Al powders with high calorific values can be used as metal fuels for propellants. Because B powder has a number of essential physical and chemical properties, such as high weight and high volumetric heating value, it has become the

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preferred metal component, especially for weapon systems that are weight and volume constrained. High-energy B-based propellants meet engine performance requirements and are an ideal choice for solid-fuel rockets, both in theoretical design and in development practice.

High fuel content fuels have a higher specific impulse because they contain metallic fuels with a high calorific value and a higher density. Be is known to have a higher heating value, but beryllium and its combustion products are highly toxic; lithium has very low density and very high activity, and Li is incompatible with many fuel components. Neither of these can be used. The main properties of the three common metals and their characteristics are summarized in Table 1. In the following, we consider B to be a "metallic" propellant component [5-14].

Table 1. Heat of explosion values of various fuels (Q is the specific heat of combustion)

Fuel	Atomic weight	Density [g/cm^3]	Melting point [°C]	Boiling point [°C]	Q [kJ/kg]	Volumetric heating values [kJ/cm^3]
B	10.81	2.35	2074	2550	58800	131.6
Graphite	12.01	2.26	3730	–	32800	73.8
Al	26.98	2.70	660	2447	31100	83.9
Mg	24.30	1.74	650	1117	24700	43.0
Titanium	47.86	4.50	1668	3287	19700	88.8
Zirconium	91.22	6.49	1855	4409	12200	78.2

However, the preparation process for fuel-rich solid propellants containing B powder is difficult due to the presence of a viscous H_3BO_3 and B_2O_3 layer on the surface of the amorphous B powder, which can react with the −OH groups of the HTPB binder [15-18]. This prevents the application of B particles in solid propellants. Hence we have introduced here highly energetic combustion agents, containing the *closo*-dodecaborate ion (Figure 1), with a high heat of combustion that can provide high-temperature combustion products and improve the propulsion performance of ducted rockets.

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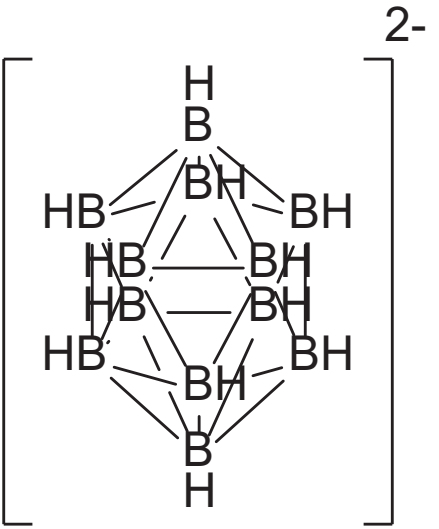

Figure 1. The molecular structure of *closo*-dodecaborate $[B_{12}H_{12}]^{2-}$ion

The most important parameter for evaluating the performance of a propellant composition is the I_{sp} values. This is the total impulse delivered per unit of propellant grain consumed. In other words, the amount of thrust delivered per unit mass flow. I_{sp} provides information about the efficiency of the solid propellant grain. In space applications, where there is no possibility to refill propellant, even a small increase in the I_{sp} value plays an important role for the flight. This is because when the gas output and the energy in the gases per propellant grain are greater, the net thrust delivered per mass flow rate increases, improving the overall performance of the vehicle.

Calculating an I_{sp} value is very tedious for compositions, as current methods involve a need to design the grain, and material of the composition and then to fire it. This requires the synthesis of the necessary materials and the preparation of the propellant strand in accordance with the various predictions that do this, and the firing and measurement of the burning rate. Furthermore, the methods for measuring the burning time are not very reliable because they could be associated with human observational errors. In addition, we cannot really measure the amount of energy released and other required parameters; these would need to be determined in a separate set of experiments.

Moreover, the number of trials needed to observe a pattern, and the amount of material that must be prepared for each trial, its preparation, and experiment would cost a lot of material, time, and human effort. In cases where we need to change the composition and have a rough idea of the outcome before we can

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actually finalise the composition, is another difficult task that requires the same amount of effort. To overcome this, we have used the EXPLO5 code [19], which allowed us to predict various fuel performance parameters without losing time or material. All we need to do is to characterize the components of the propellant grain and then check for different compositions.

2 Materials

We considered the following ionic salts:

- 3,3′-(but-2-yne-1,4-diyl)*bis*(1-methyl-1H-imidazol-3-ium)dodecaborate (BAM-H1),
- *bis*(triethylammonium)dodecaborate (BAM-H2),
- *bis*(butylmethylimidazolium)dodecahydroborate (BAM-H3).

Other borane-containing salts, ammonium dodecahydrododecaborate (ADDB) and triethylammonium dodecahydrododecaborate (TEDDB), had been tested [20].

The molecular structures of BAM-H1, BAM-H2 and BAM-H3 are shown in Figure 2. They act as the fuel. We chose hydroxyl-terminated polybutadiene (HTPB) as the binder and ammonium chlorate(VII) (NH_4ClO_4, AP) as the oxidant. HTPB and AP are the conventional combination of binder and oxidant, and so we checked the performance of the fuel blends. The percentage of binder was set to 14%, the ratio of fuel to oxidizer was varied and the performance was checked. The input parameters of the fuel components in EXPLO5 are density and heats of formation. The density values of the fuel components BAM-H1, BAM-H2 and BAM-H3 were determined by the gas pycnometer method. The experimental enthalpy of formation (ΔH_f) and enthalpy of combustion (ΔH_c) was determined by burning the fuel component in an oxygen bomb calorimeter to determine the enthalpy of combustion, followed by correcting the enthalpy of combustion and determination of ΔH_f by Hess's thermochemical equation (Table 2). We have already published the complete synthetic procedure, characterization, and determination of ΔH_f in the literature [21, 22].

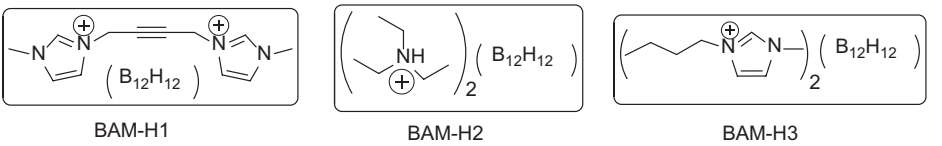

Figure 2. Molecular structures of BAM-H1, BAM-H2 and BAM-H3

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Table 2. Experimental properties of the tested *closo*-dodecaborate salts

Fuel	Molecular formula	Melting point [°C]	T_d [°C]	ΔH_c [kJ/mol]	ΔH_f [kJ/mol]	Q [kJ/kg]	IS [J]	FS [N]
BAM-H1	$C_{12}H_{28}N_4B_{12}$	228	232	–15493.4	–811.9	–43264.4	>50	>360
BAM-H2	$C_{12}H_{44}N_2B_{12}$	268	270-275	–15338.6	–3253.3	–44303.1		
BAM-H3	$C_{16}H_{42}N_4B_{12}$	217	270-275	–19134.4	–745.8	–45529.8		

T_d is the decomposition temperature, IS is the impact sensitivity and FS is the friction sensitivity

A binder is a polymeric compound that can combine with other components of the propellant into a whole mass with optimal performance. Although binders account for only 10-15% of the mass fraction in solid propellants, they play an important role. On the one hand, they can be used as an energy-rich propellant component to produce CO_2 and H_2O through treatment with oxidants to generate thrust; on the other hand, they can facilitate the uniform bonding of metal additives, oxidants and combustion modifiers to form solid grains that have some potency at both high and low temperatures, form a continuous medium in fuel-rich B-based propellants, and provide combustible elements such as C and H to release energy during combustion.

Binders widely used in recent years include high polymers such as HTPB and glycidyl azide polymer (GAP), which are inexpensive, have near-Newtonian fluid mobility with low viscosity, and allow the addition of other solid components. The structural formula of HTPB is shown in Figure 3.

$$HO-\left(H_2C-HC=CH-CH_2\right)_n-OH$$

Figure 3. The molecular structures of HTPB

The oxidizer is an essential component of fuel-rich propellants. It can provide the oxygen required for combustion and control the combustion rate of the fuel by increasing the particle size. The selection of oxidizers is based on the principle of high effective oxygen content, high specific gravity and high ΔH_f, gaseous products and physical and chemical stability during processing and storage. At present, AP is a widely used oxidizer, which has excellent overall performance (such as heat of formation, effective oxygen content, density, *etc.*).

3 EXPLO5 Version 6.03 Calculations

EXPLO5 applies the free energy minimization method and calculates the products [19]. The products are estimated from the basic compositions, their respective

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proportions in the output are given, and the energies involved are calculated accordingly. The gaseous products are determined by the equation of state for ideal gases, while the condensed products (if any) are considered incompressible. The energies contained in the respective equations are determined by Hess's law. The respective exhaust gas velocities (V_E), the combustion temperatures and I_{sp}, which are among the parameters of a fuel to be considered, were calculated.

The density, ΔH_f and molecular formulas are the input parameters for the software. The density of all three *closo*-dodecaborate salts was determined using a gas pycnometer and reported as 1.0000 g/cm^3. The experimental enthalpy of formation of all three *closo*-dodecaborate salts were determined using a bomb calorimeter. The ΔH_f values of BAM-H1, BAM-H2, and BAM-H3 are listed above in Table 2.

The calculations of Isp were carried out under isobaric combustion conditions at a chamber pressure of 7 MPa compared to ambient pressure, with equilibrium expansion conditions at the nozzle throat. The calculations were performed with different formulations of BAM-H1, BAM-H2 and BAM-H3 as fuel components, AP as oxidant and HTPB as binder and the results are listed in Tables 3-5. The specific impulse of amorphous B and Al as fuels and AP as oxidizer and HTPB as binder were also determined with different compositions for comparison, and the results are listed in Tables 6 and 7. In these Tables, T_c means the isobaric combustion temperature.

Table 3. Predicted properties of a propellant with 14% HTPB binder and BAM-H1

BAM-H1 [%]	AP [%]	T_c [K]	I_{sp} [s]	V_E [m/s]
6	80	2477.1	236.52	2320.3
7	79	2401.9	235.34	2308.7
8	78	2327.0	234.25	2297.9
9	77	2253.3	233.26	2288.3
10	76	2178.5	232.39	2279.7
11	75	2127.5	231.64	2272.4
12	74	2118.0	230.80	2264.2
13	73	2108.2	229.94	2255.7
14	72	2099.8	229.18	2248.3
15	71	2095.2	228.54	2242.0
16	70	2101.1	228.32	2239.9
17	69	2102.2	228.77	2244.2
18	68	2096.7	229.27	2249.1
19	67	2078.0	229.35	2249.9
20	66	2048.3	228.61	2242.7

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Table 4. Predicted properties of a propellant with 14% HTPB binder and BAM-H2

BAM-H2 [%]	AP [%]	T_c [K]	I_{sp} [s]	V_E [m/s]
6	80	2216.2	227.81	2234.9
7	79	2103.6	225.23	2209.5
8	78	2008.0	222.87	2186.3
9	77	1966.5	220.48	2162.9
10	76	1919.6	217.53	2133.9
11	75	1867.8	215.67	2115.7
12	74	1811.6	213.48	2094.2
13	73	1752.0	211.58	2075.6
14	72	1694.2	209.87	2058.9
15	71	1649.4	208.43	2044.7
16	70	1631.9	207.30	2033.7
17	69	1642.6	206.44	2025.2
18	68	1670.7	205.81	2018.9
19	67	1700.3	205.35	2014.5
20	66	1723.7	205.05	2011.5

Table 5. Predicted properties of a propellant with 14% HTPB binder and BAM-H3

BAM-H3 [%]	AP [%]	T_c [K]	I_{sp} [s]	V_E [m/s]
6	80	2476.7	240.60	2360.3
7	79	2403.9	240.18	2356.2
8	78	2333.9	239.95	2354.0
9	77	2264.0	239.80	2352.5
10	76	2194.5	239.73	2351.8
11	75	2152.6	239.80	2352.5
12	74	2147.9	239.93	2353.7
13	73	2143.0	240.01	2354.5
14	72	2140.1	239.69	2351.3
15	71	2140.4	240.21	2356.5
16	70	2147.7	240.55	2359.8
17	69	2158.2	241.44	2368.5
18	68	2150.8	242.60	2379.9
19	67	2124.1	243.47	2388.4
20	66	2092.2	243.65	2390.2

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Table 6. Predicted properties of a propellant with 14% HTPB binder and amorphous B powder

B [%]	AP [%]	T_c [K]	I_{sp} [s]	V_E [m/s]
6	80	2812.2	248.55	2438.3
7	79	2787.7	249.35	2446.1
8	78	2758.5	250.24	2454.9
9	77	2721.3	251.28	2465.1
10	76	2664.2	252.46	2476.6
11	75	2555.1	252.98	2481.7
12	74	2491.2	250.35	2455.9
13	73	2491.2	250.35	2455.9
14	72	2468.6	244.73	2400.8
15	71	2455.3	241.76	2371.7
16	70	2441.0	238.72	2341.9
17	69	2424.8	235.57	2310.9
18	68	2407.0	232.30	2278.8
19	67	2386.9	228.91	2245.6
20	66	2364.7	225.45	2211.7

Table 7. Predicted properties of a propellant with 14% HTPB binder and Al powder

Al [%]	AP [%]	T_c [K]	I_{sp} [s]	V_E [m/s]
6	80	3080.9	251.02	2462.5
7	79	3110.1	255.26	2504.1
8	78	3169.5	256.54	2516.7
9	77	3196.7	257.62	2527.3
10	76	3223.0	258.65	2537.3
11	75	3248.4	259.61	2546.8
12	74	3272.6	260.52	2555.7
13	73	3295.4	261.35	2563.8
14	72	3317.3	262.14	2571.6
15	71	3337.1	262.84	2578.4
16	70	3354.6	263.46	2584.6
17	69	3369.0	263.99	2589.7
18	68	3380.1	264.43	2594.0
19	67	3386.3	264.70	2596.7
20	66	3386.6	264.75	2597.2

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4 Discussion

From Table 1, it can be seen that B, Al, and Mg powder fuels each have their own advantages and disadvantages. As far as energy use is concerned, Al has the highest density at 2.70 g·cm^{-3}, B the second highest, and Mg the lowest at 1.74 g·cm^{-3}. As for combustion, the melting and boiling points of Mg, Al and B successively increase, and the combustion difficulties also increase. The melting points of Mg and Al are low and are around 660 °C, while the melting point of B can be as high as 2074 °C. The boiling points of Al and B are similar, and the boiling point of B can reach up to 2550 °C, while Mg has a minimum boiling point of 1117 °C.

In Table 1, the value of Q of Al is 31100 kJ/kg, and that of B is 58800 kJ/kg. After comprehensive consideration of factors such as energy performance and combustion characteristics, B powder was selected as the main metallic propellant additive; while a small amount of Mg powder or Al powder was added to provide fuel-rich propellants with good ignition performance. However, the practical energy result of B powder was much lower than the theoretical value, about 39000 kJ/kg, which was due to incomplete combustion and a coating of B_2O_3 layer on the surface. This prevents the availability of unburned B powder during combustion. Besides, there is another problem: B powder is not easy to ignite; it needs ultra-pure oxygen, which is not possible in practice. For this reason, newly developed and prepared next-generation rocket propellant fuels were introduced, such as BAM-H1, BAM-H2, and BAM-H3. The energy release of these compounds was about 45000 kJ/kg (Table 2), which is higher than the practically released energy of B powder. After the combustion process, there are no unburned B particles. Therefore, these salts are potential candidates for use as fuel, fuel additive and/or burn-rate accelerators.

Using the above input parameters (Tables 3-7), the I_{sp} values of the corresponding propellant compositions were determined. The HTPB binder was fixed at 14%, the percentage of the salt propellant component was varied from 6% to 20%, the percentage of the oxidant from 80% to 66%, all adding up to 100%. Following the same pattern, the calculation of I_{sp} was carried out for the three fuel components BAM-H1, BAM-H2 and BAM-H3 individually, as well as for amorphous B powder and Al. For each fuel component, we calculated 15 experiments with fuel content ranging from 6% to 20%, as shown in Tables 3-7. B-containing compositions produce a large number of condensed products, which leads to convergence problems. To address this problem, some of the following compounds, produced in very small amounts, such as $B(OH)_3$(s), $B_3H_3O_3$(s), BHO_2(s), B_4C(s), B_4C(l), BN(s), B(s), and C(gr, s), were removed in the

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calculation process. As condensed products, only the following products B_2O_3(s), B_2O_3(l), B(l), BN, BH_2, BCl, BCl_3, B, B_2O_3, $B(OH)_3$, BO_2, BO, BHO_2, CO, H_2, H_2O, HCl, N_2, CO_2, H, Cl, NH_3, NO, HCN, Cl_2, CClO, CHNO, NH_2, CH_4, ClO, N, CNO, CH_2Cl_2, C_2H_4, N_2H_4, C_2H_6, $CHCl_3$ were considered in order to obtain a uniform dependence of I_{sp} and V_E on the percentage of BAM-H1, BAM-H2 and BAM-H3, and the percentage of B in the total propellant composition.

In Table 3, BAM-H1 shows an I_{sp} value of 236.52 s for the composition of 6% BAM-H1, 80% AP and 14% HTPB. In Table 4, BAM-H2 shows a higher I_{sp} value at 227.81 s for the composition of 6% BAM-H2, 80% AP and 14% HTPB. In Table 5, BAM-H3 shows the highest specific impulse value at 243.65 s for the composition of 20% BAM-H3, 66% AP and 14% HTPB. In Table 6, B powder shows the highest I_{sp} value at 252.98 s for a composition of 11% B powder, 75% AP and 14% HTPB.

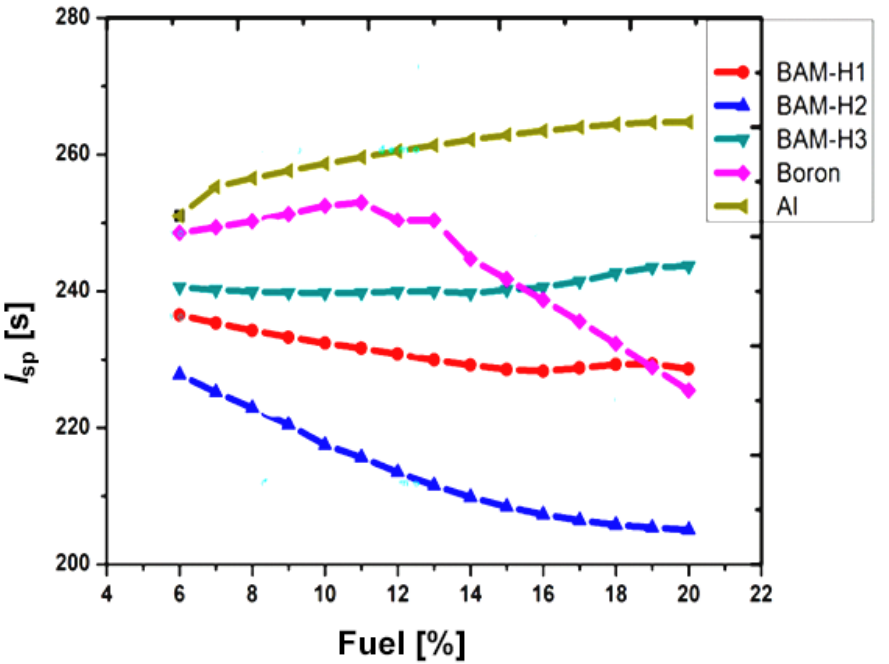

Figure 4. Summary of the data from Tables 3-6 for I_{sp}

As can be seen from the comparative diagram Figure 4, the initial percentage of 6% of the fuel BAM-H1 gave the highest value of I_{sp} at 236.52 s. After increasing the percentage from 6% to 20%, no great progress was made. Similarly, BAM-H2 also gave its highest value of I_{sp} at 227.81 s at only 6%;

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further addition of the fuel did not give a higher value of I_{sp}. Compared to these two fuels, BAM-H3 had the highest value of I_{sp} from a low percentage of 6% to 20%. The addition of fuel amount increased the I_{sp} value and reached the highest value at 20% of 243.65 s. While the addition of B powder as a fuel from 6% to 11% increased the I_{sp} value from 248.55 to 252.98 s, the I_{sp} value decreased from 11% to 20% on further addition of B fuel. In the case of Al fuel, the I_{sp} value increased from 6% to 20% and reaches its highest I_{sp} value of 264.75 s. Finally, of the three new fuels, BAM-H3 achieved very good I_{sp} value, higher than the other two, BAM-H1 and BAM-H2.

4 Conclusions

- Theoretically determined I_{sp} values were obtained for different combinations of propellant compositions of three *closo*-dodecaborate ($[B_{12}H_{12}]^{2-}$) salts, with AP as the oxidant and 14% HTPB as the binder. Taken into consideration were the *closo*-dodecaborate salts:
  - 3,3′-(but-2-yne-1,4-diyl) *bis*(1-methyl-1*H*-imidazol-3-ium) dodecaborate (BAM-H1),
  - *bis*(triethylammonium)dodecaborate (BAM-H2), and
  - *bis*(butylmethylimidazolium)dodecahydroborate (BAM-H3).
- The results have shown that all three *closo*-dodecaborate salts in the corresponding propellant compositions achieve high I_{sp} values, compared to the relevant propellant compositions with B and Al powders as fuel.
- Introduction of *closo*-dodecaborate salts creates no problems with combustion, agglomeration and aggregation, however this article shows the importance and potential use of *closo*-dodecaborate salts as components in propellant compositions. Further experimental evaluations are needed to bring this potential to reality.
- The results of this study may be helpful in the development of new high-energy materials for propellant and explosive applications.

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