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Supporting Information

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Research paper

Ammonium Dodecahydrododecaborate $(NH_4)_2[B_{12}H_{12}]$: Hydrogen and Boron Rich Fuel for Jet Propulsion Engines

Pandurang M. Jadhav[1)], Jay Patil[2)], Hima Prasanth[1)], Gururaja Rao[1)]
[1)] *High Energy Materials Research Laboratory, Pune 411021, India*
[2)] *Institute of Chemical Technology, Indian Oil Odisha Campus, Bhubaneswar 751073, India*
* *E-mail:* jadhav.pm.hemrl@gov.in

Content

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1 Elemental Analysis

Elemental analysis was performed on a VarioMICRO instrument. Elemental analysis showed N 14.74 and H 10.16%, which were close to the theoretical figures, ($N_2H_{20}B_{12}$: MW 177.72; requires N:15.75% and H: 11.1%). Moreover, no carbonaceous matter was found in the elemental analysis which indicated complete conversion of triethylammonium dodecahydrododecaborate to ADDB.

2 Thermal Analysis

Differential Scanning Calorimetry (DSC), and Thermo-Gravimetric (TGA) analysis of ADDB were done on a PerkinElmer thermal analyzer (STA 6000) under a nitrogen atmosphere at 10^{o}C/min heating rate. Figure S1(a) shows an endothermic peak at 310 ^{o}C, of 1497 J/g. The decomposition of ADDB was also reported to be 310 ^{o}C by Ivanov *et al.* [15]. This supported the formation of ADDB using the new synthesis route. On the other hand, TGA showed weight gains in two stages (Figure S1(b)). A 15% weight gain was observed in the range 300-600 ^{o}C, and a significant weight gain (39%) was seen between 600 and 1000 ^{o}C.

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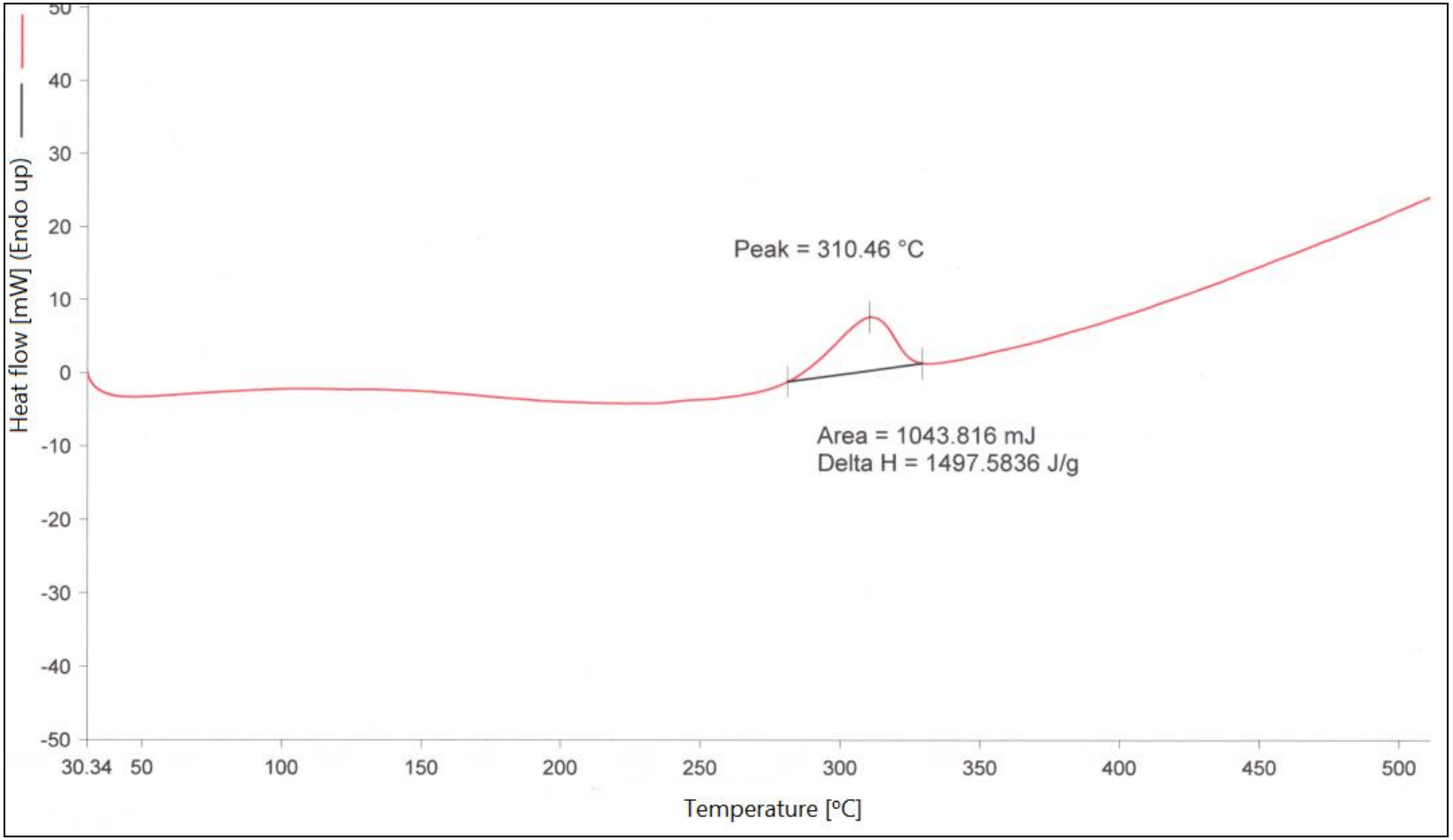

(a)

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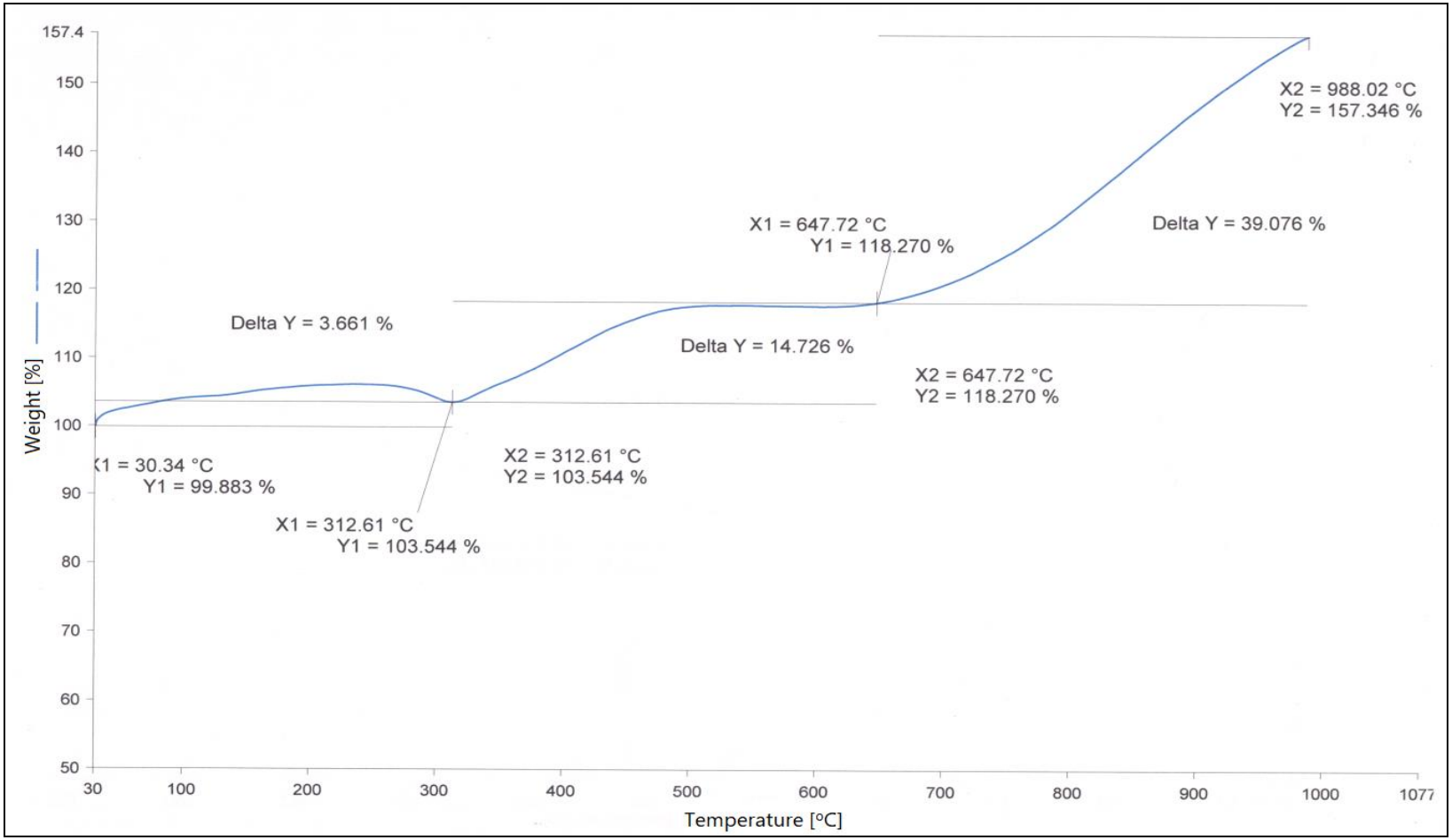

(b)

Figure S1. (a) DSC and (b) TGA of ADDB

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3 Spectroscopic Analysis

Fourier transform infrared spectra (FTIR) were recorded on a Nicolet iS50 FTIR Spectrometer of Thermo Fisher Scientific, which is shown in Figure S2. The FTIR analysis showed strong peaks at:

– 3231 cm^{-1} (NH_4^+),

– 2468 cm^{-1} (B–H),

– 1401 cm^{-1} (N–H), and

– 1070 cm^{-1} (B–B),

which confirmed the functional groups of ADDB.

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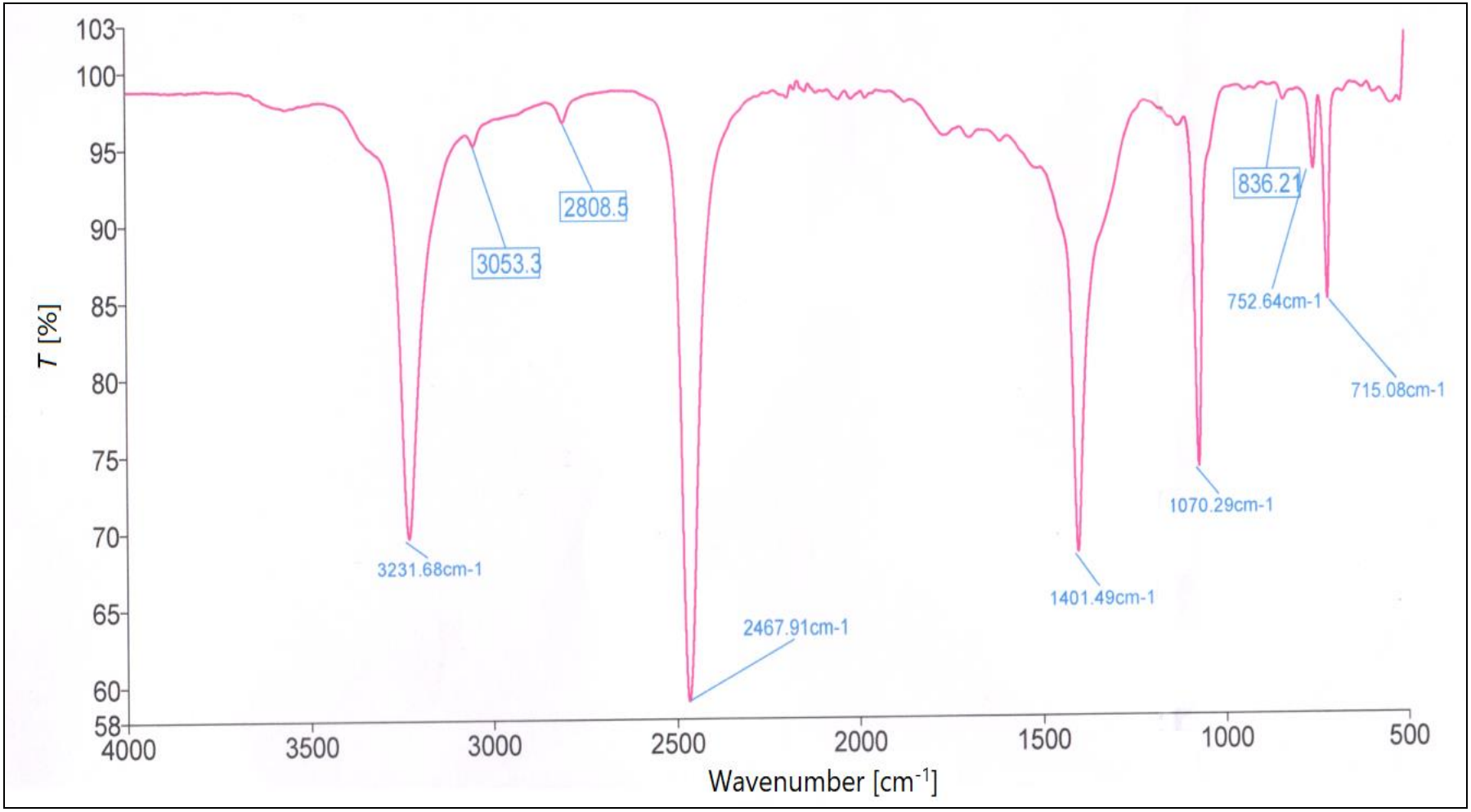

Figure S2. FT-IR spectrum of ADDB

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Nuclear magnetic resonance (NMR) spectral analysis of ADDB was carried out in DMSO solution. ^{1}H and ^{11}B spectra were recorded on a Bruker MSL-300 instrument. ^{1}H NMR exhibited hydrogen peaks at 7.09 (s, NH_4) and 1.14 (q, B–H) ppm. ^{11}B NMR showed the boron peak at 15 (d, B) ppm.

4 CEA Details

Theoretical rocket performance, assuming equilibrium composition during expansion from an infinite area combustor, was computed using the NASA-GLENN Chemical Equilibrium Program (CEA2) [13]. The oxidizer to fuel problem was solved for various ratios and fuels at a fixed equilibrium temperature of 3800 K, an inside pressure of 70 bar and a pressure ratio of 20. The enthalpy from an inbuilt library was used for all ingredients except ADDB and TEDDB. The input file format was as follows.

Problem: oxidizer (o)/fuel (f)

Rocket equilibrium: t_{cset} = 3800 K

p =70 bar,

p_i/p = 20

Ingredient details:

Fuel = JP-10	Enthalpy: h = –122.8 kJ/mol
Oxidizer = Air	Enthalpy: h = –0.129 kJ/mol
Fuel = ADDB	Enthalpy: h = –668.47 kJ/mol
Fuel = TEDDB	Enthalpy: h = –3204.73 kJ/mol
Fuel = HTPB	Enthalpy: h = –0.26 kJ/mol
Oxidizer = AP	Enthalpy: h = –295.77 kJ/mol

In case of the JP-10 compositions, the effect of additional fuel i.e. boron and boranes, on the flame temperature was computed and provided as follows.

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Table S1. Effect of boron and boranes on the flame temperature of JP-10

Fuel (Composition in %)	Flame temperature [K]
JP-10 (50%)	1103.4
JP-10 (40%) and TEDDB (10%)	1183.2
JP-10 (40%) and ADDB (10%)	1429.9
JP-10 (40%) and boron (10%)	3096.4

References (Cited according to the main part of this paper)

[13] McBride, B.; Gordon, G., *Chemical Equilibrium Program CEA2: NASA Glenn Research Center, Cleveland, OH; 2004.* Report NASA RP-1311, Part I, **1994**.

[15] Ivanov, S.V.; Miller, S.M.; Anderson, O.P.; Solntsev, K.A.; Strauss, S.H. Synthesis and Stability of Reactive Salts of Dodecafluoro-closo-dodecaborate(2−). *J. Am. Chem. Soc.* **2003**, *125*(16): 4694-4695.

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