

Supporting Information

Synthesis and Ignition Properties Research of 1,5-Diazabicyclo[3.1.0]Hexane Type Compounds As Potential Green Hypergolic Propellants

Table S1 ^1H NMR, EI and Element Analysis Results of DABHCs

	^1H NMR δ (400 MHz, CDCl_3)	EI (m/z)	Element analysis (%)
<i>DABH:</i>	3.3 (2H, -N-CH-C-), 3.0 (2H, -N-CH-C-),		calculated: C 57.11 H
	2.5 (1H, -N-CH-N-), 2.2 (1H, -N-CH-N-), [M-1] $^{+}$ 83.0	9.59 N 33.30; found: C	
<i>MDABH:</i>	1.8 (1H, -C-CH-C-), 1.7 (1H, -C-CH-C-)	56.89 H 9.60 N 33.51	
	3.3 (2H, -N-CH-C-), 3.0 (2H, -N-CH-C-),		calculated: C 61.19 H
<i>EDABH:</i>	2.3 (1H, -N-CH-N-), 1.7 (2H, -C-CH-C-), [M-1] $^{+}$ 97.1	10.27 N 28.54; found: C	
	1.2 (3H, -CH ₃)	62.08 H 10.09 N 27.83	
<i>DDABH:</i>	3.4 (2H, -N-CH-C-), 3.0 (2H, -N-CH-C-),		calculated: C 64.24 H
	2.2 (1H, -N-CH-N-), 1.8 (2H, -C-CH-C-), [M-1] $^{+}$ 111.1	10.78 N 24.97; found: C	
	1.5 (2H, -CH-C-), 1.0 (3H, -CH ₃)	65.05 H 10.59 N 24.36	
	3.2 (2H, -N-CH-C-), 2.8 (2H, -N-CH-C-),		calculated: C 64.24 H
	2.3 (1H, -C-CH-C-), 2.0 (1H, -C-CH-C-), [M-1] $^{+}$ 111.1	10.78 N 24.97; found: C	
	1.3 (3H, -CH ₃), 1.2 (3H, -CH ₃)	64.71 H 10.80 N 24.49	

Table S2 Purities of DABH under Different Rectification Conditions

Time/h	Packing	Temperature /°C	Purity/%
6	--	70	-
6	--	80	83
12	--	80	86
24	--	80	91
48	--	80	91

96	--	80	91
144	--	80	91
48	exist	80	91

Table S3 Purities of DABH under Different Column Chromatography Conditions [†]

Moving phase	Purity/%
Petroleum ether/ethyl acetate=20:1	81
Petroleum ether/ethyl acetate=4:1	81
Chloroform/methyl alcohol = 24:1	87
Dichloromethane/methyl alcohol = 5:1	99

[†]The stationary for chromatography was silica gel.