Supporting Information

Effects of *closo*-Icosahedral Periodoborane Salts on Hypergolic Reaction of 70% H_2O_2 with Energetic Ionic Liquid

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Experimental Section

General

All commercially available reagents were used without further purification. ^{1}H, $^{13}C\{H\}$, and ^{11}B NMR spectra were measured on a Bruker Avance III 400 MHz nuclear magnetic resonance spectrometer. DMSO-d_6 and acetone-d_6 were used as solvent. FTIR spectra were recorded using an ATR unit on a Bruker Tensor 27 spectrometer. Densities were measured at 25 ° C by employing a Micromeritics AccuPyc 1330 gas pycnometer. Single crystal X-ray diffraction data were collected at 123 K on Rigaku Compact HomeLab diffractometer, equipped with a Saturn 944 HG CCD detector and Oxford Cryostream cooling system, using monochromatic Cu-Ka radiation (1.54178 a) from a MicroMaxTM-003 sealed tube microfocus X-ray source. Ignition tests were filmed with a high-speed Phantom v610 camera, operated at 20,000 frames·sec^{-1}.

Synthesis

$[Cs]_2[B_{12}I_{12}]$ (2).[1] A mixture of $Cs_2B_{12}H_{12}$ (0.10 g, 0.26 mmol) and I_2 (2.11 g, 8.31 mmol) in glacial acetic acid (10 mL) was heated at 250 °C for 5 days in a sealed glass reactor (20 mL). After that time, the reaction mixture was cooled to RT and quenched with aqueous solution of Na_2SO_3 (1.8 g in 50 mL of water) to give a clear yellow solution that was filtered to remove black solid particles. After slow evaporation of the resulted solution at RT, colorless crystals of pure $Cs_2B_{12}I_{12}$ (92% yield) were obtained. ^{11}B NMR (acetone-d_6) δ: –15.7.

$[Cu^{II}(en)_2(CH_3CN)_2^{2+}][B_{12}I_{12}^{2-}]$ (4). To a solution of $[Et_4N]_2[B_{12}I_{12}]$ **3** (97.0 mg, 0.05 mmol) in CH_3CN (3 mL) an aqueous solution of bis(ethylenediamine)copper(II) dihydroxide solution (1.0 M in H_2O) was added dropwise at RT, until dark blue colored solution was obtained. After slow evaporation of this solution at RT, dark blue crystals of pure $[Cu(en)_2(CH_3CN)_2^{2+}][B_{12}I_{12}^{2-}]$ **4** (78% yield) were obtained. FTIR (ATR): ν 3779, 3699, 3578, 3406, 3278, 3226, 3116, 2938, 2881, 2359, 2108, 1566, 1490, 1405, 1137, 1082, 1015, 924, 674, 619, 522, 412 cm^{-1}. Elemental analysis: calcd. (%) for $C_8H_{22}B_{12}CuI_{12}N_6$ (1,920.10): C 5.01; H 1.16; N 4.38; found: C 4.81; H 2.21; N 4.68.

$[FcCH_2NEtMe_2^+]_2[B_{12}I_{12}^{2-}]$ (5). To a solution of $[Cs]_2[B_{12}I_{12}]$ **2** (100 mg, 0.05 mmol) in water (3 mL) a solution of $[FcCH_2NEtMe_2^+][I^-]^2$ (45.7 mg, 0.11 mmol) in water (2 mL) was added dropwise at RT and the reaction mixture was stirred for 30 min. After completion of the reaction, the yellow solid product was collected by filtration and dried at ambient temperature. Later the solid was dissolved in acetonitrile and slow evaporation of the solvent at RT, brown crystals of pure $[FcCH_2NEtMe_2^+]_2[B_{12}I_{12}^{2-}]$ **5** (82% yield) were obtained. ^{1}H NMR (400 MHz, DMSO-d_6) δ: 1.26 (s, 3H), 2.82 (s, 6H), 3.17 (q, 2H), 3.32 (q, 2H), 4.25 (m, 4H), 4.35-4.38 (m, 4H), 4.49 (s, 2H). ^{13}C NMR (100 MHz, DMSO-d_6) δ: 7.89, 48.36, 58.09, 63.53, 69.0, 69.97, 71.94, 72.93. ^{11}B NMR (128 MHz, DMSO-d_6) δ: 15.46. FTIR (ATR): ν 3899, 3838, 3743, 3677, 3647, 3617, 3565, 3078, 2920, 2854, 2315, 1743, 1699, 1649, 1541, 1516, 1459, 1373, 1234, 1192, 1103, 1045, 1027, 996, 926, 827, 799, 713, 480 cm^{-1}. Elemental analysis: calcd. (%) for $C_{30}H_{44}B_{12}Fe_2I_{12}N_2$ (2,199.20): C 16.40; H 2.02; N 1.28; found: C 16.23; H 2.85; N 1.73.

NMR and FTIR Spectroscopy.

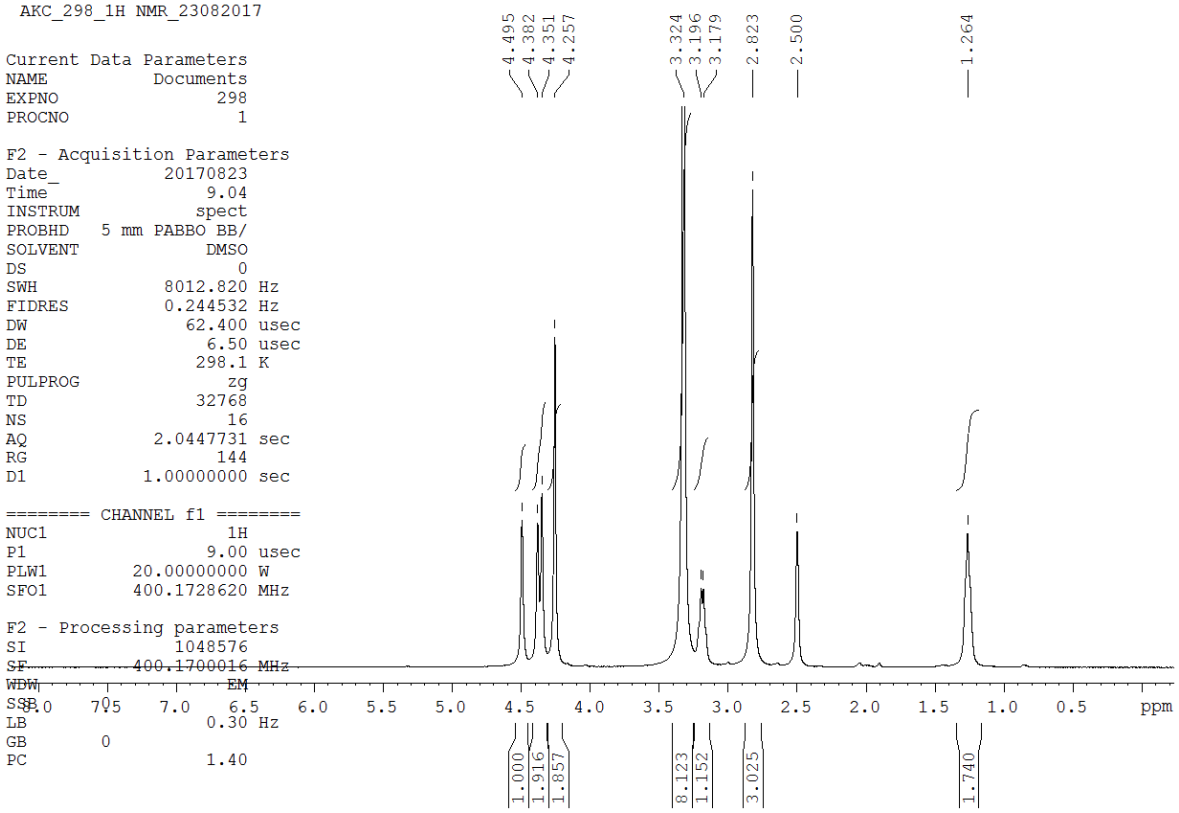


Figure S1. ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of $[FcCH_2NEtMe_2^+]_2[B_{12}I_{12}^{2-}]$ promoter **5.**

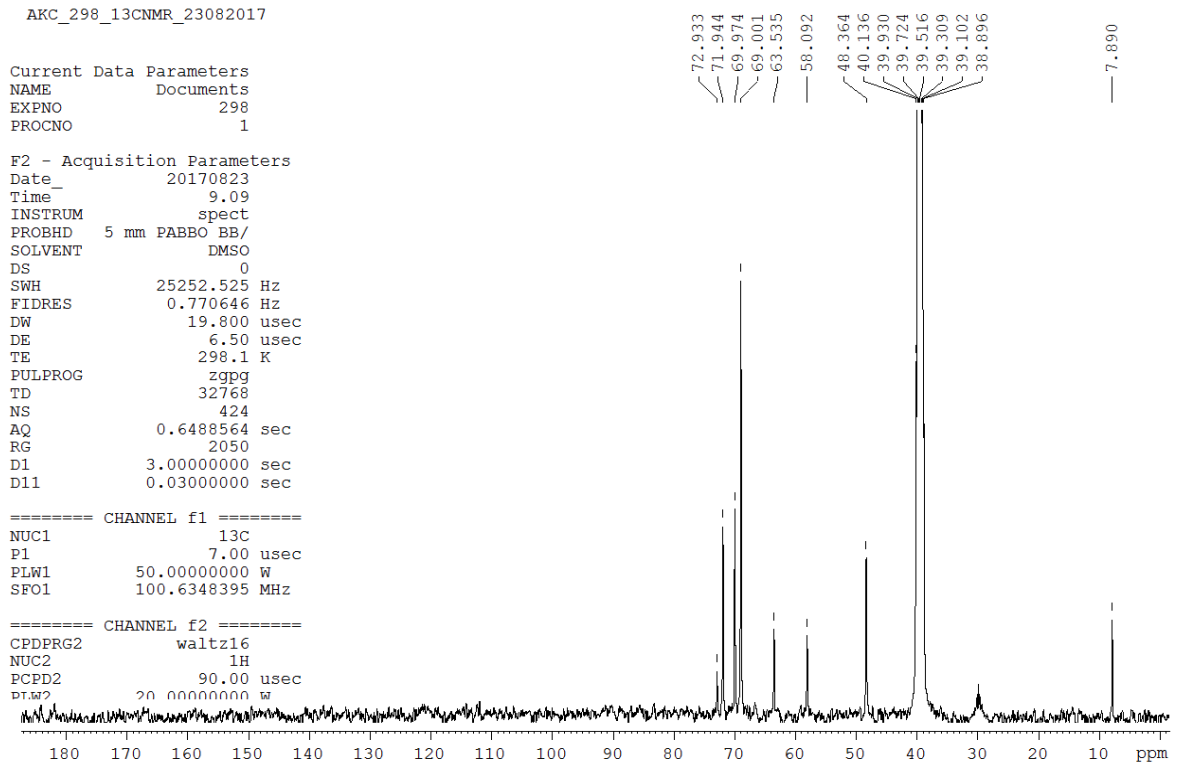


Figure S2. ^{13}C NMR (100 MHz, DMSO-d_6) spectrum of $[FcCH_2NEtMe_2^+]_2[B_{12}I_{12}^{2-}]$ promoter **5.**

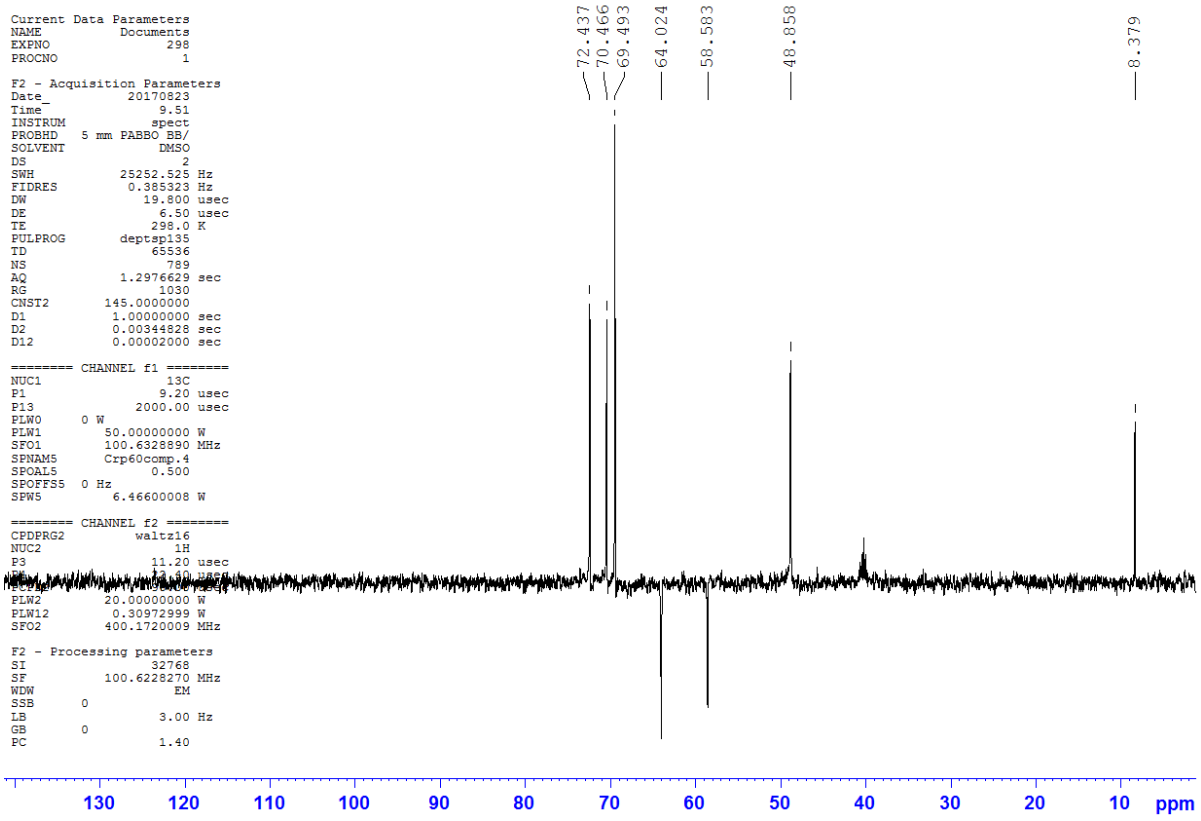


Figure S3. ^{13}C DEPT-135 (400 MHz, DMSO-d_6) spectrum of $[FcCH_2NEtMe_2^+]_2[B_{12}I_{12}^{2-}]$ promoter **5.**

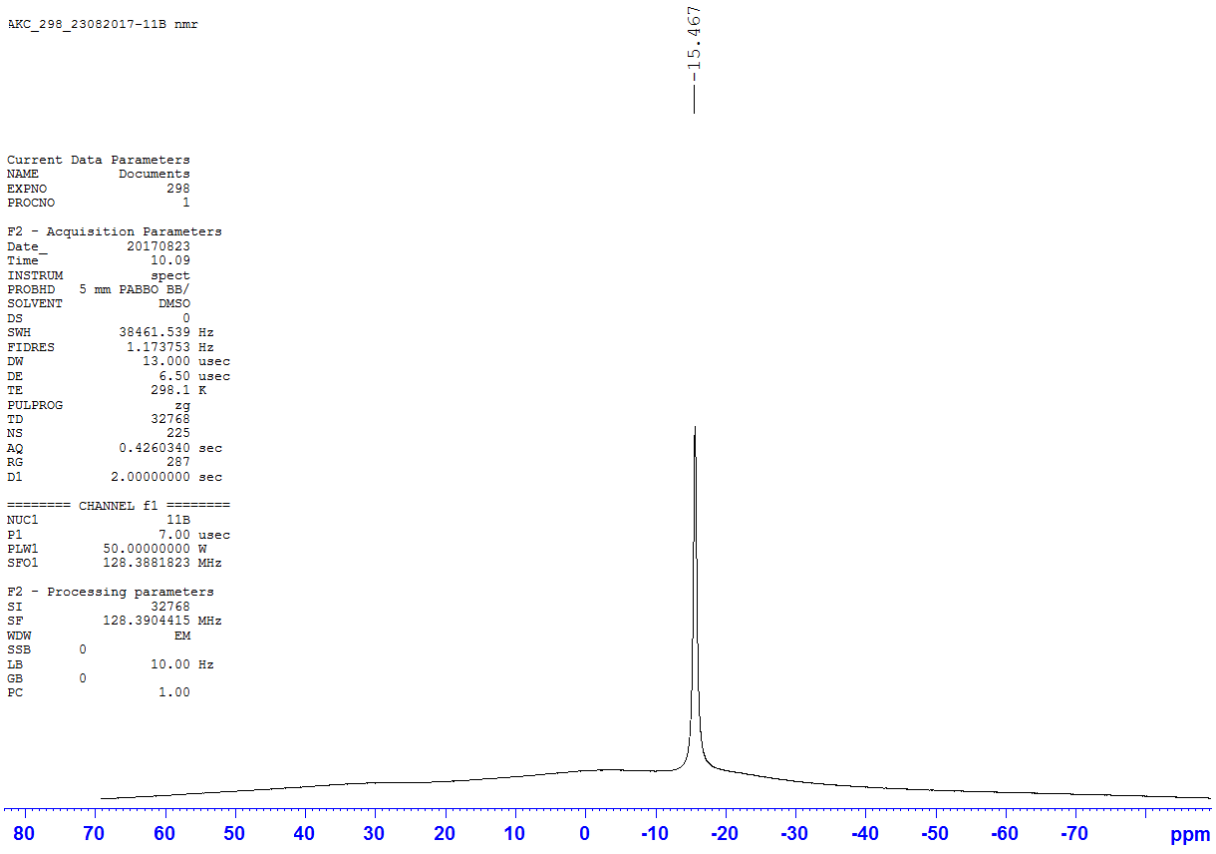


Figure S4. ^{11}B NMR (128 MHz, DMSO-d_6) spectrum of $[FcCH_2NEtMe_2^+]_2[B_{12}I_{12}^{2-}]$ promoter **5.**

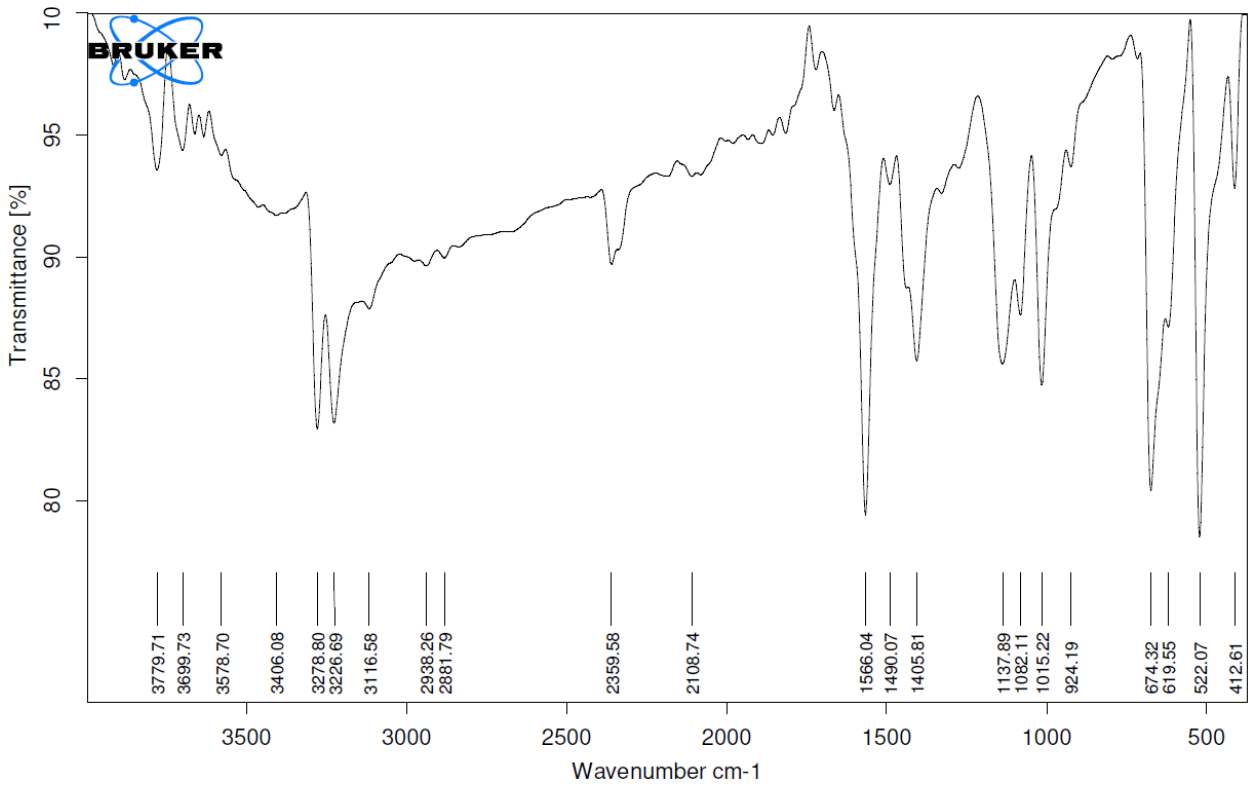


Figure S5. FTIR spectrum of $[Cu(en)_2(CH_3CN)_2^{2+}][B_{12}I_{12}^{2-}]$ promoter **4.**

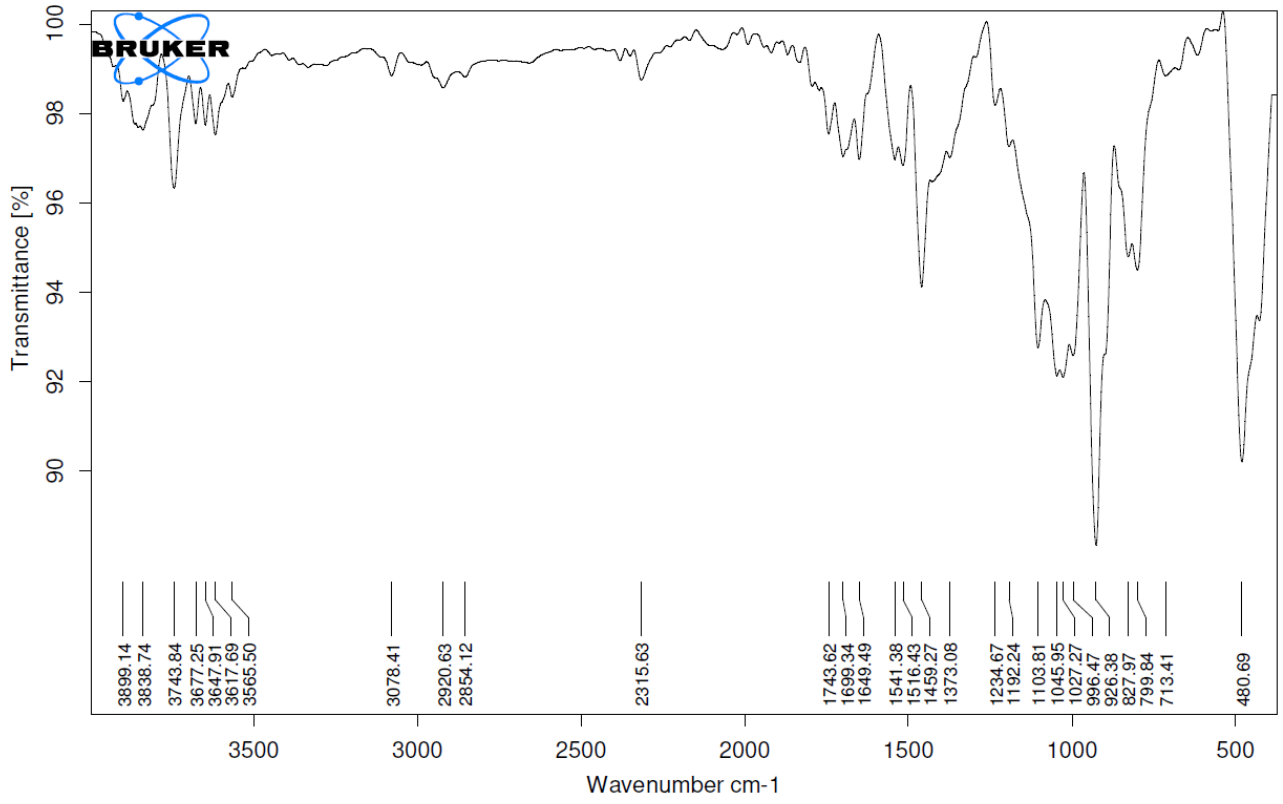


Figure S6. FTIR spectrum of $[FcCH_2NEtMe_2^{+}]_2[B_{12}I_{12}^{2-}]$ promoter **5.**

X-ray Crystallography

Table S1. X-ray crystallography details.

	Promoter 4 (CCDC 1590191)	**Promoter 5** (CCDC 1590192)
Formula	$B_{12}I_{12}C_8H_{22}CuN_6$	$B_{12}I_{12}2(C_{15}H_{22}FeN)$
FW/g·mol^{-1}	1,918.39	2,196.89
Color	dark blue	brown
Crystal size/mm	0.257 × 0.120 × 0.060	0.200 × 0.200 × 0.100
Crystal system	monoclinic	triclinic
Space group	*C2/m*	*P-1*
a/Å	16.9343 (14)	10.9499 (4)
b/Å	12.3926 (10)	12.0570 (5)
c/Å	11.3050 (9)	12.3471 (4)
α/°	90	61.337 (1)
β/°	120.836 (2)	69.030 (1)
γ/°	90	81.237 (1)
V/Å^3	2037.1 (3)	1335.24 (9)
$P_{calcd.}$/g.mol^{-3}	3.128	2.732
T/K	110 (2)	110 (2)
F(000)	1674	986
μ/ mm^{-1}	9.645	7.507
Absorption correction	multi-scan	multi-scan
h, k, lmax	22, 16, 15	14, 16, 16
θ range/°	2.098; 28.394	1.925; 28.463
Nref	2656	6683
Parameters	102	265
Data completeness	0.993	0.988
R(reflections)	0.0161 (2560)	0.0214 (6307)
wR2(reflections)	0.0345 (2656)	0.0509 (6683)

Table S2. Bond lengths in promoters **4** and **5**.

Bond length (Å)		
Promoter **4**	Promoter **5**	
I1 B1 2.170(3)	I1 B1 2.168(3)	B4 B6 1.798(5)
Cu1 N2 2.008(2)	Fe1 C15 2.028(3)	I5 B5 2.167(3)
Cu1 N2 2.008(2)	Fe1 C13 2.031(3)	B5 B3 1.784(5)
Cu1 N2 2.008(2)	Fe1 C14 2.037(3)	B5 B6 1.794(5)
Cu1 N2 2.008(2)	Fe1 C7 2.041(3)	B5 B2 1.795(5)
B1 B2 1.785(4)	Fe1 C8 2.042(3)	I6 B6 2.174(3)
B1 B1 1.786(6)	Fe1 C11 2.042(3)	B6 B3 1.791(5)
B1 B3 1.791(4)	Fe1 C10 2.042(3)	B6 B4 1.798(5)
B1 B4 1.792(4)	Fe1 C16 2.043(3)	C7 C11 1.421(5)
B1 B4 1.792(4)	Fe1 C12 2.045(3)	C7 C8 1.422(5)
I2 B2 2.156(4)	Fe1 C9 2.049(3)	C8 C9 1.414(5)
N2 C3 1.477(4)	B1 B6 1.786(5)	C9 C10 1.419(5)
B2 B1 1.786(4)	B1 B2 1.790(5)	C10 C11 1.418(5)
B2 B3 1.785(6)	B1 B3 1.793(5)	C12 C13 1.420(5)
B2 B4 1.792(4)	B1 B5 1.795(5)	C12 C16 1.422(5)
B2 B4 1.792(4)	B1 B4 1.797(5)	C13 C14 1.434(5)
I3 B3 2.160(4)	I2 B2 2.160(3)	C14 C15 1.434(4)
C3 C3 1.509(5)	B2 B6 1.787(5)	C15 C16 1.433(4)
B3 B4 1.791(4)	B2 B4 1.793(5)	C15 C17 1.494(4)
B3 B4 1.791(4)	B2 B5 1.795(5)	C17 N18 1.529(4)
B3 B1 1.791(4)	B2 B3 1.799(5)	N18 C20 1.497(4)
B3 B1 1.791(4)	I3 B3 2.167(3)	N18 C19 1.502(4)
I4 B4 2.157(3)	B3 B5 1.784(5)	N18 C21 1.520(4)

N4 C5 1.130(6)	B3 B4 1.787(5)	C21 C22 1.504(5)
B4 B1 1.792(4)	B3 B6 1.791(5)	
B4 B1 1.792(4)	I4 B4 2.164(3)	
B4 B4 1.793(6)	B4 B5 1.792(5)	
C5 C6 1.462(7)	B4 B2 1.793(5)	

Table S3. Bond angles in promoters **4** and **5**.

Bond angle (º)		
Promoter **4**	Promoter **5**	
N2 Cu1 N2 95.95(1)	C15 Fe1 C13 69.46(1)	B1 B3 I3 120.8(2)
N2 Cu1 N2 84.05(1)	C15 Fe1 C14 41.32(1)	B2 B3 I3 122.1(2)
N2 Cu1 N2 180.00(9)	C13 Fe1 C14 41.29(1)	B3 B4 B5 107.9(2)
N2 Cu1 N2 180.0	C15 Fe1 C7 154.06(1)	B3 B4 B2 107.7(2)
N2 Cu1 N2 84.05(1)	C13 Fe1 C7 125.56(1)	B5 B4 B2 60.08(2)
N2 Cu1 N2 95.95(1)	C14 Fe1 C7 163.40(1)	B3 B4 B1 60.05(2)
B2 B1 B1 59.99(1)	C15 Fe1 C8 164.36(1)	B5 B4 B1 60.01(2)
B2 B1 B3 108.0(2)	C13 Fe1 C8 105.22(1)	B2 B4 B1 108.1(2)
B1 B1 B3 60.10(1)	C14 Fe1 C8 125.24(1)	B3 B4 B6 59.94(2)
B2 B1 B4 108.1(2)	C7 Fe1 C8 40.75(1)	B5 B4 B6 107.7(2)
B1 B1 B4 108.17(1)	C15 Fe1 C11 120.17(1)	B2 B4 B6 59.69(2)
B3 B1 B4 59.96(1)	C13 Fe1 C11 164.48(1)	B1 B4 B6 108.0(2)
B2 B1 B4 60.10(1)	C14 Fe1 C11 153.80(1)	B3 B4 I4 122.5(2)
B1 B1 B4 108.17(1)	C7 Fe1 C11 40.72(1)	B5 B4 I4 120.8(2)
B3 B1 B4 108.0(2)	C8 Fe1 C11 68.63(1)	B2 B4 I4 121.6(2)
B4 B1 B4 60.04(2)	C15 Fe1 C10 109.11(1)	B1 B4 I4 121.1(2)
B2 B1 I1 120.90(2)	C13 Fe1 C10 151.95(1)	B6 B4 I4 122.8(2)
B1 B1 I1 121.92(8)	C14 Fe1 C10 118.85(1)	B3 B5 B4 108.2(2)
B3 B1 I1 122.74(2)	C7 Fe1 C10 68.22(1)	B3 B5 B6 60.07(2)
B4 B1 I1 121.93(2)	C8 Fe1 C10 68.27(1)	B4 B5 B6 108.1(2)
B4 B1 I1 120.82(2)	C11 Fe1 C10 40.64(1)	B3 B5 B2 60.36(2)
C3 N2 Cu1 108.84(1)	C15 Fe1 C16 41.22(1)	B4 B5 B2 59.99(2)
B1 B2 B1 60.0(2)	C13 Fe1 C16 68.99(1)	B6 B5 B2 108.5(2)
B1 B2 B3 108.2(2)	C14 Fe1 C16 69.30(1)	B3 B5 B1 107.8(2)
B1 B2 B3 108.2(2)	C7 Fe1 C16 119.24(1)	B4 B5 B1 60.14(2)
B1 B2 B4 60.13(1)	C8 Fe1 C16 152.10(1)	B6 B5 B1 59.71(2)
B1 B2 B4 108.2(2)	C11 Fe1 C16 109.36(1)	B2 B5 B1 108.1(2)
B3 B2 B4 60.08(1)	C10 Fe1 C16 129.42(1)	B3 B5 I5 122.7(2)
B1 B2 B4 108.2(2)	C15 Fe1 C12 68.99(1)	B4 B5 I5 120.2(2)
B1 B2 B4 60.13(1)	C13 Fe1 C12 40.76(1)	B6 B5 I5 122.9(2)
B3 B2 B4 60.08(1)	C14 Fe1 C12 68.96(2)	B2 B5 I5 120.8(2)
B4 B2 B4 108.3(3)	C7 Fe1 C12 107.43(2)	B1 B5 I5 121.6(2)
B1 B2 I2 121.53(2)	C8 Fe1 C12 117.21(1)	B1 B6 B2 60.10(2)
B1 B2 I2 121.53(2)	C11 Fe1 C12 128.10(2)	B1 B6 B3 107.9(2)
B3 B2 I2 121.7(2)	C10 Fe1 C12 166.80(3)	B2 B6 B3 107.8(2)
B4 B2 I2 121.58(1)	C16 Fe1 C12 40.70(1)	B1 B6 B5 60.18(2)
B4 B2 I2 121.58(1)	C15 Fe1 C9 127.65(1)	B2 B6 B5 108.1(2)
N2 C3 C3 106.64(2)	C13 Fe1 C9 116.77(1)	B3 B6 B5 59.70(2)
B2 B3 B4 60.13(1)	C14 Fe1 C9 106.60(1)	B1 B6 B4 108.0(2)
B2 B3 B4 60.13(1)	C7 Fe1 C9 68.21(1)	B2 B6 B4 60.02(2)
B4 B3 B4 108.4(3)	C8 Fe1 C9 40.44(1)	B3 B6 B4 59.72(2)
B2 B3 B1 108.0(2)	C11 Fe1 C9 68.44(1)	B5 B6 B4 107.6(2)
B4 B3 B1 108.0(2)	C10 Fe1 C9 40.60(1)	B1 B6 I6 121.6(2)
B4 B3 B1 60.03(1)	C16 Fe1 C9 166.82(1)	B2 B6 I6 122.2(2)
B2 B3 B1 108.0(2)	C12 Fe1 C9 150.86(1)	B3 B6 I6 121.6(2)
B4 B3 B1 60.03(15)	B6 B1 B2 59.96(1)	B5 B6 I6 121.2(2)
B4 B3 B1 108.0(2)	B6 B1 B3 108.0(2)	B4 B6 I6 122.3(2)
B1 B3 B1 59.8(2)	B2 B1 B3 60.28(1)	C11 C7 C8 108.2(3)

B2 B3 I3 119.2(2)	B6 B1 B5 60.11(1)	C11 C7 Fe1 69.7(2)
B4 B3 I3 120.74(2)	B2 B1 B5 107.9(2)	C8 C7 Fe1 69.66(2)
B4 B3 I3 120.74(2)	B3 B1 B5 107.4(2)	C9 C8 C7 108.0(3)
B1 B3 I3 123.83(2)	B6 B1 B4 108.2(2)	C9 C8 Fe1 70.06(2)
B1 B3 I3 123.83(2)	B2 B1 B4 108.2(2)	C7 C8 Fe1 69.59(2)
B3 B4 B2 59.79(2)	B3 B1 B4 59.68(1)	C8 C9 C10 108.0(3)
B3 B4 B1 60.00(2)	B5 B1 B4 59.85(1)	C8 C9 Fe1 69.50(3)
B2 B4 B1 107.7(2)	B6 B1 I1 121.7(2)	C10 C9 Fe1 69.44(2)
B3 B4 B1 107.7(2)	B2 B1 I1 121.5(2)	C11 C10 C9 108.4(3)
B2 B4 B1 59.77(2)	B3 B1 I1 121.8(2)	C11 C10 Fe1 69.68(2)
B1 B4 B1 107.75(2)	B5 B1 I1 122.1(2)	C9 C10 Fe1 69.97(2)
B3 B4 B4 107.99(2)	B4 B1 I1 121.7(2)	C10 C11 C7 107.5(3)
B2 B4 B4 107.80(2)	B6 B2 B1 59.93(2)	C10 C11 Fe1 69.69(2)
B1 B4 B4 59.99(2)	B6 B2 B4 60.29(2)	C7 C11 Fe1 69.6(2)
B1 B4 B4 59.98(2)	B1 B2 B4 108.1(2)	C13 C12 C16 108.6(3)
B3 B4 I4 120.82(2)	B6 B2 B5 108.1(2)	C13 C12 Fe1 69.07(2)
B2 B4 I4 122.87(2)	B1 B2 B5 107.8(2)	C16 C12 Fe1 69.58(2)
B1 B4 I4 120.31(2)	B4 B2 B5 59.93(2)	C12 C13 C14 108.2(3)
B1 B4 I4 123.49(2)	B6 B2 B3 107.8(2)	C12 C13 Fe1 70.17(2)
B4 B4 I4 121.73(8)	B1 B2 B3 59.97(2)	C14 C13 Fe1 69.61(2)
N4 C5 C6 178.6(6)	B4 B2 B3 107.5(2)	C13 C14 C15 107.4(3)
	B5 B2 B3 59.53(2)	C13 C14 Fe1 69.11(2)
	B6 B2 I2 123.1(2)	C15 C14 Fe1 69.01(1)
	B1 B2 I2 122.3(2)	C16 C15 C14 108.0(3)
	B4 B2 I2 122.1(2)	C16 C15 C17 124.3(3)
	B5 B2 I2 120.5(2)	C14 C15 C17 127.5(3)
	B3 B2 I2 121.0(2)	C16 C15 Fe1 69.95(1)
	B5 B3 B4 108.5(2)	C14 C15 Fe1 69.67(2)
	B5 B3 B6 60.23(2)	C17 C15 Fe1 122.5(2)
	B4 B3 B6 60.35(2)	C12 C16 C15 107.8(3)
	B5 B3 B1 108.1(2)	C12 C16 Fe1 69.72(2)
	B4 B3 B1 60.26(2)	C15 C16 Fe1 68.83(2)
	B6 B3 B1 108.5(2)	C15 C17 N18 114.3(3)
	B5 B3 B2 60.11(2)	C20 N18 C19 108.4(3)
	B4 B3 B2 108.2(2)	C20 N18 C21 110.7(2)
	B6 B3 B2 108.4(2)	C19 N18 C21 108.0(2)
	B1 B3 B2 59.75(2)	C20 N18 C17 108.2(2)
	B5 B3 I3 122.7(2)	C19 N18 C17 109.0(2)
	B4 B3 I3 120.4(2)	C21 N18 C17 112.4(2)
	B6 B3 I3 121.6(2)	

Hirshfeld Surface Analyses

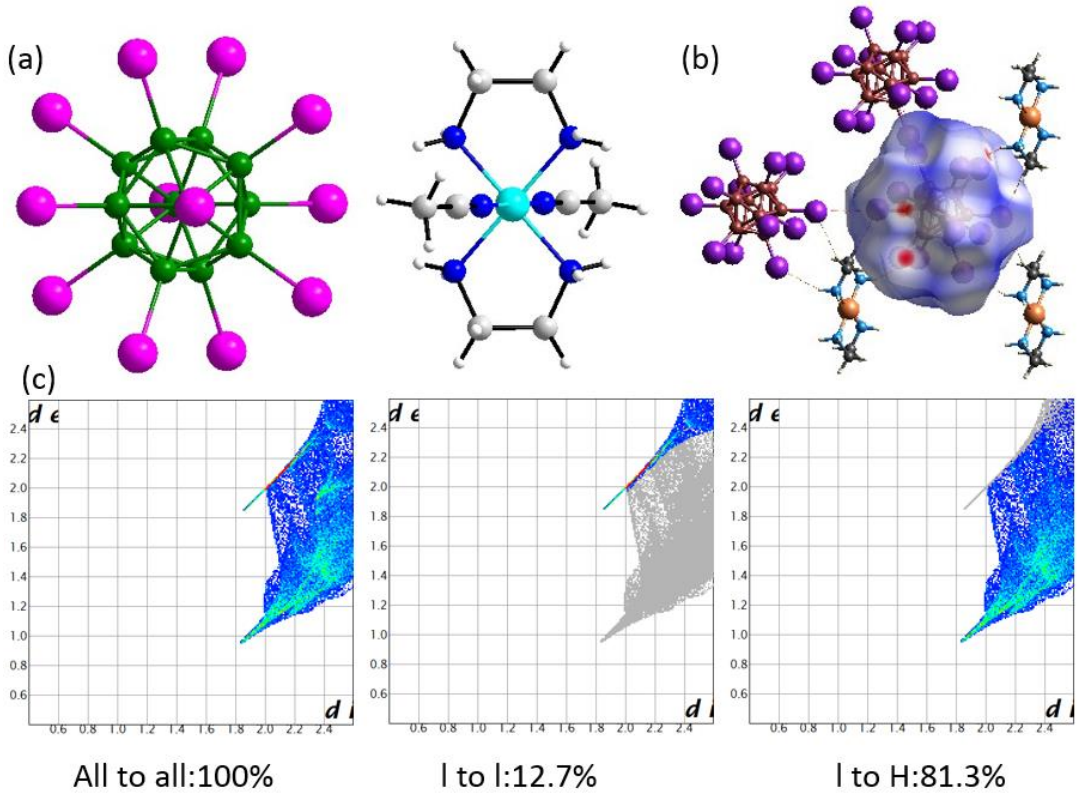


Figure S7. (a) Molecular structure of promoter **4**; (b) a calculated Hirshfeld surface of **4** in the crystal structure; (c) fingerprint plots of the Hirshfeld analysis of intermolecular interactions in the crystal of **4** (I···I, and; I···H interactions).

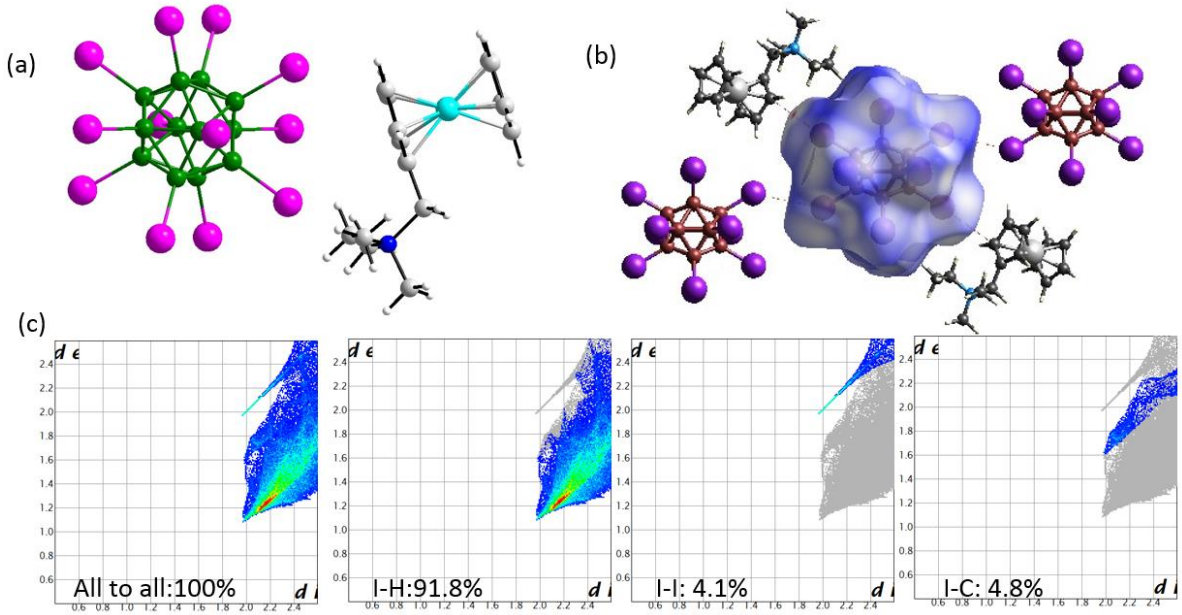


Figure S8. (a) Molecular structure of promoter **5**; (b) a calculated Hirshfeld surface of **5** in the crystal structure; (c) fingerprint plots of the Hirshfeld analysis of intermolecular interactions in the crystal of **5** (I···I, and; I···H interactions).

Ignition Tests and Related Analyses

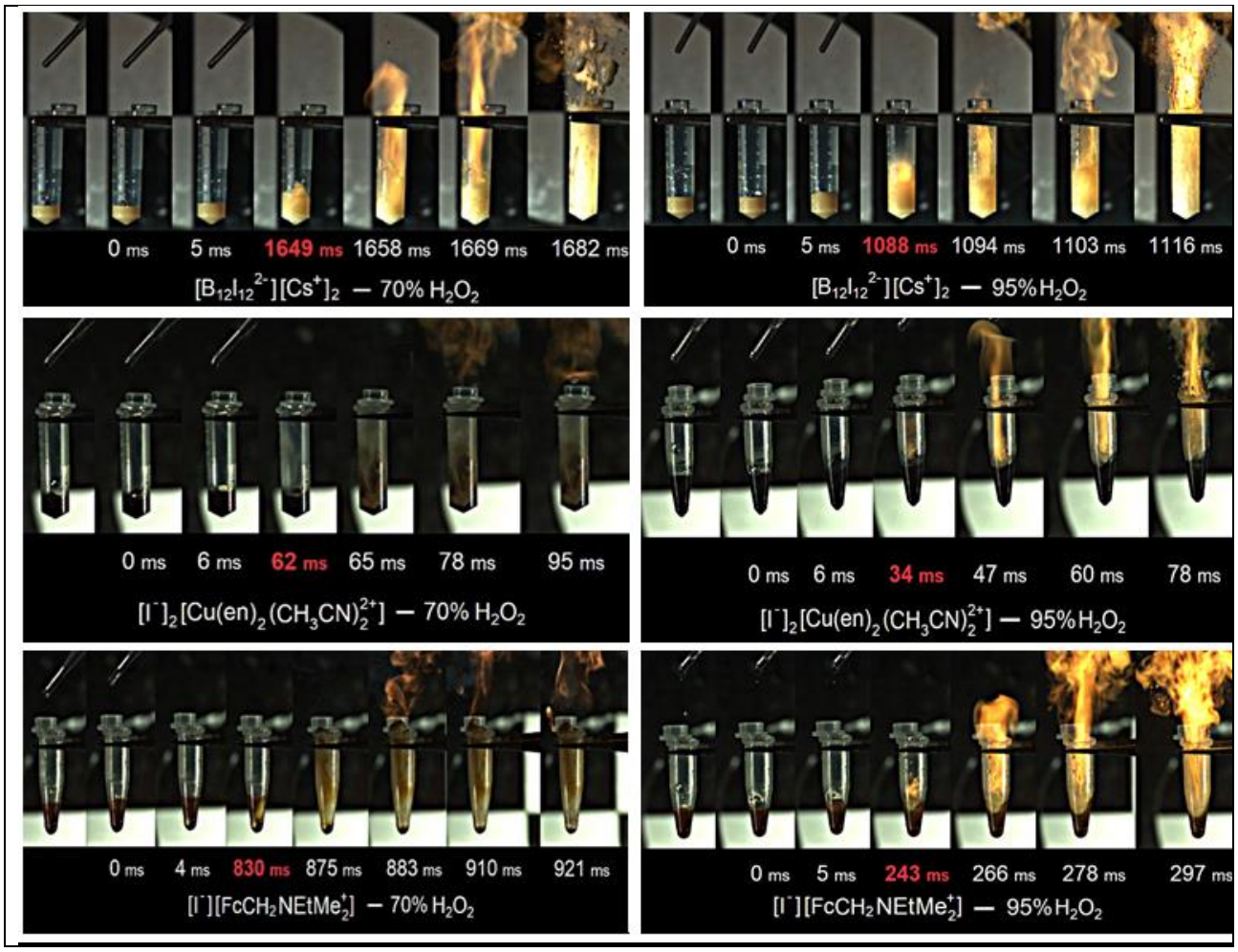


Figure S9. Selected frames from conducted hypergolic ignition experiments. The time in the frames containing the first signs of ignition is colored in red.

Promoter 5 Conc. (wt.%)	**ID (ms)**
2.0	32
5.0	24
8.0	17
10.0	14
15.0	11

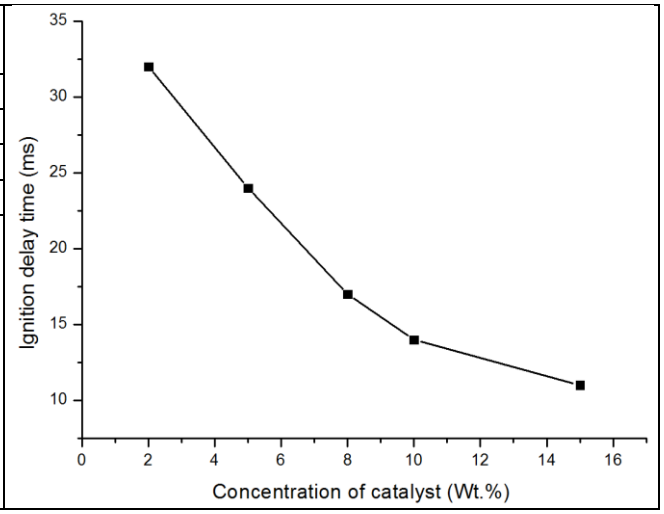


Figure S10. ID times measured in hypergolic ignition experiments in which H_2O_2 (95%) is added to [$EMIM^+$][H_3BCN^-] (oxidizer-to-fuel drop addition), while the concentration of promoter **5** is variated.

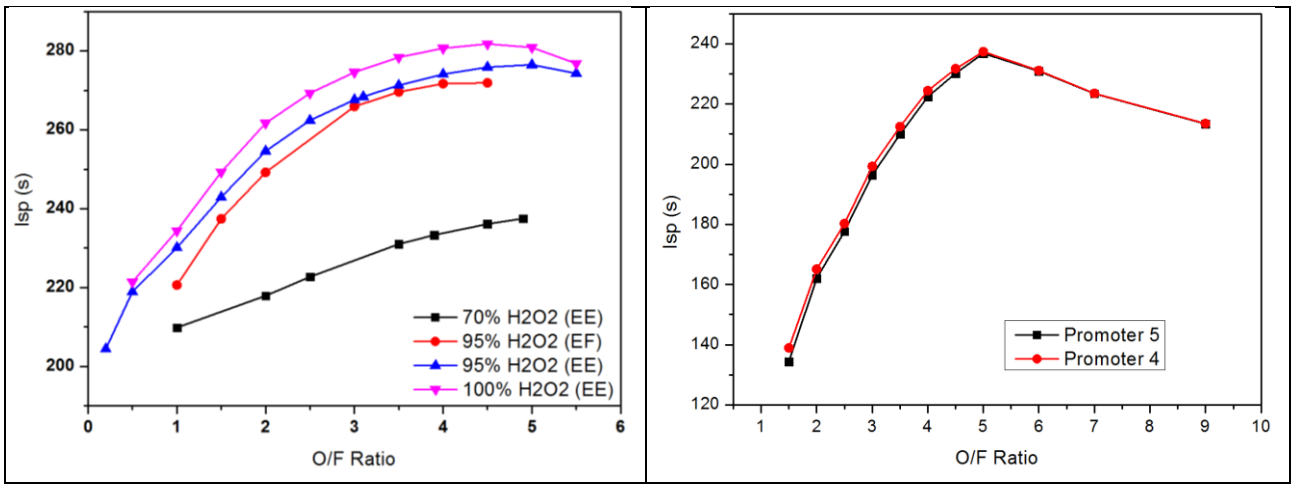


Figure S11. (*left*): Specific impulse calculations for H_2O_2 (95%) and promoter-free [EMIM][BH3CN] bi-propellant system (for more data, see pages 2-132 in the attached document entitled "Raw Data of Thermo-chemical Calculations"); (*right*): Specific impulse calculations for H2O2 (95%) and [EMIM][BH3CN] containing promoter 4 (8 wt.%) and promoter 5 (8 wt.%) bi-propellant systems (for more data, see pages 133-190 and 191-247, respectively, in the attached document entitled "Raw Data of Thermochemical Calculations").

We attempted to detect a possible emission of hydrogen from mixtures of $[EMIM^+][H_3BCN^-]$ with H_2O_2 (30%; in order to slow down the hypergolic ignition reaction) without presence of promoters, by using an insertion of a burning wooden stick into the reaction vessel containing a mixture of both reaction components. No flash flame or detonation sound that would correspond to the presence of hydrogen-oxygen mixture, was detected. Subsequently, we conducted experiments in which $[Cs^+]_2[B_{12}I_{12}^{2-}]$ promoter **2** was reacted with H_2O_2 (30%), without addition of $[EMIM^+][H_3BCN^-]$ fuel, as shown in Figures S10 and S11. Notably, mixtures of promoters **2**, **4** and **5** with $[EMIM^+][H_3BCN^-]$ were found to be stable for several weeks.

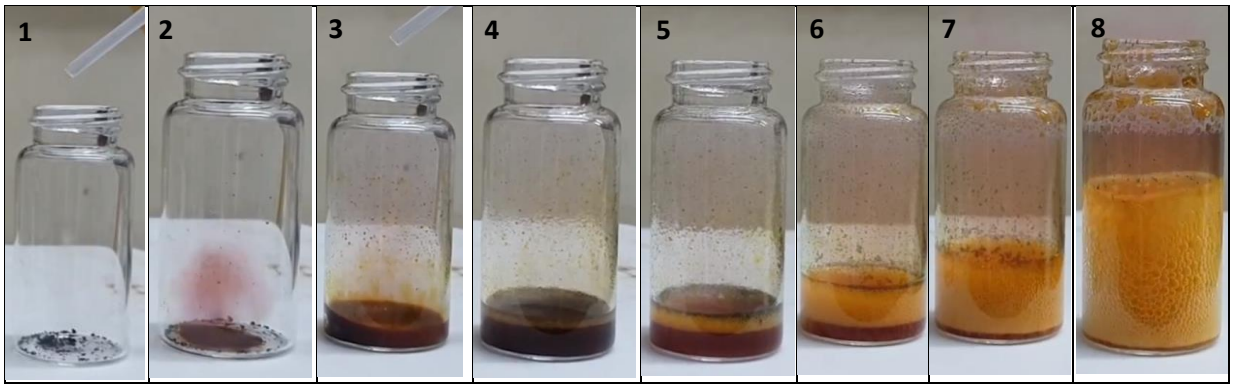


Figure S12. Reaction of $[Cs^+]_2[B_{12}I_{12}^{2-}]$ promoter **2** with H_2O_2 (30%).

1. Powder of promoter **2** (10 mg) *prior* to addition of H_2O_2.
2. Picture of promoter **2** after addition of the two drops of H_2O_2, there is a clear emission of I_2 vapors.[3] indicating a decomposition of promoter **2** upon reaction with H_2O_2.
3. Picture of promoter **2** after addition of 1.0 mL of H_2O_2.
4. Picture of promoter **2** after addition of 1.5 mL (in total) of H_2O_2.
5. Monitoring the reaction progress (from picture 5 to picture 8) between promoter **2** and H_2O_2. Emitted gas is O_2 as detected by larger scale "wooden stick" combustion experiments (Figure 2).

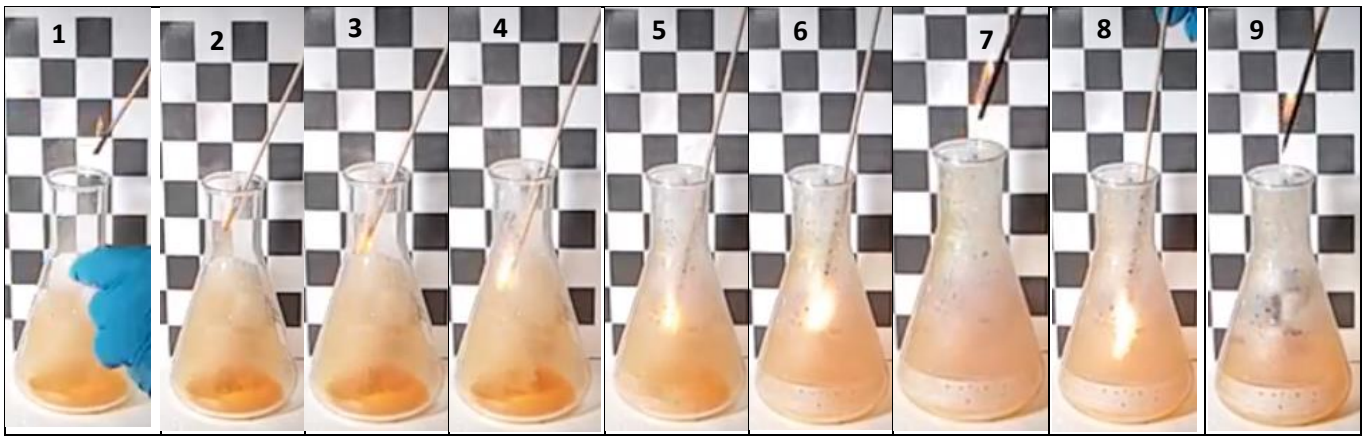
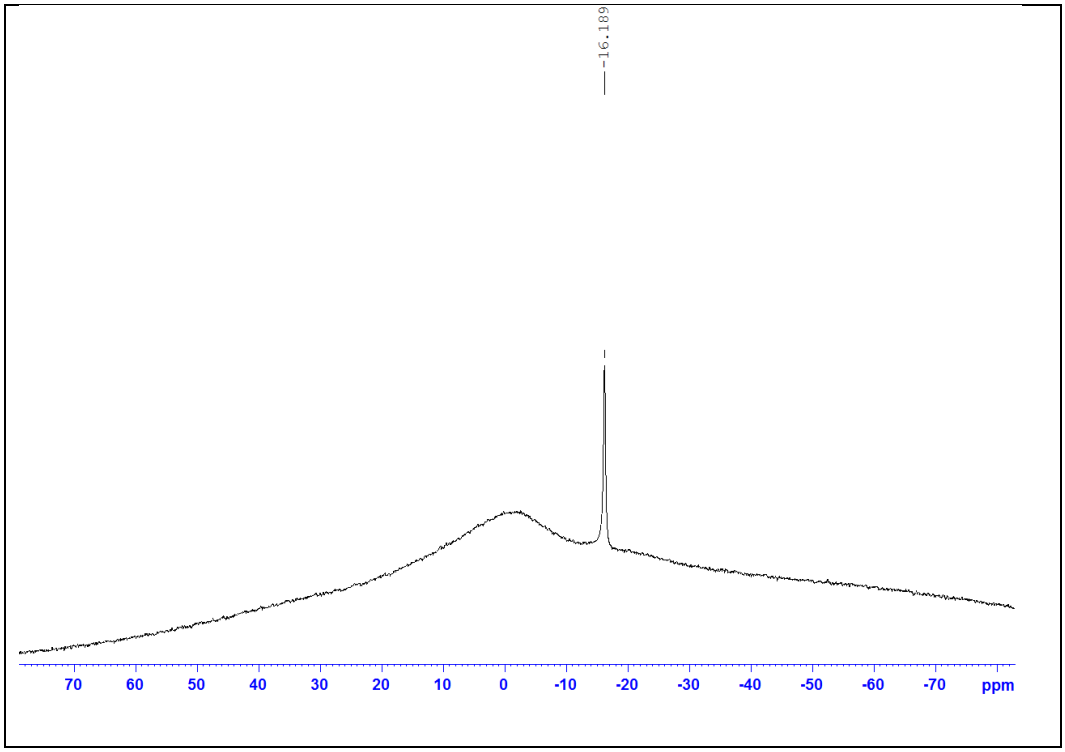


Figure S13. Reaction of $[Cs^+]_2[B_{12}I_{12}^{2-}]$ promoter **2** with H_2O_2 (30%). O_2 emission in the reaction flask was detected by the difference in the observed combustion intensity (*versus* combustion under atmospheric conditions) of burning wooden stick, inserted into the reaction vessel in which reaction of promoter **2** with H_2O_2 (30%) took place. Frames 4, 5, 6 and 8 are clearly showing much stronger combustion of a wooden stick inside the reaction vessel.

^{11}B NMR of the products of promoter **2** reaction with H_2O_2 (30%) showed a wide hump and disappearance of a sharp peak at -16.2 ppm, which is indicative to the presence of $[B_{12}I_{12}^{2-}]$ anion (Figure S12).



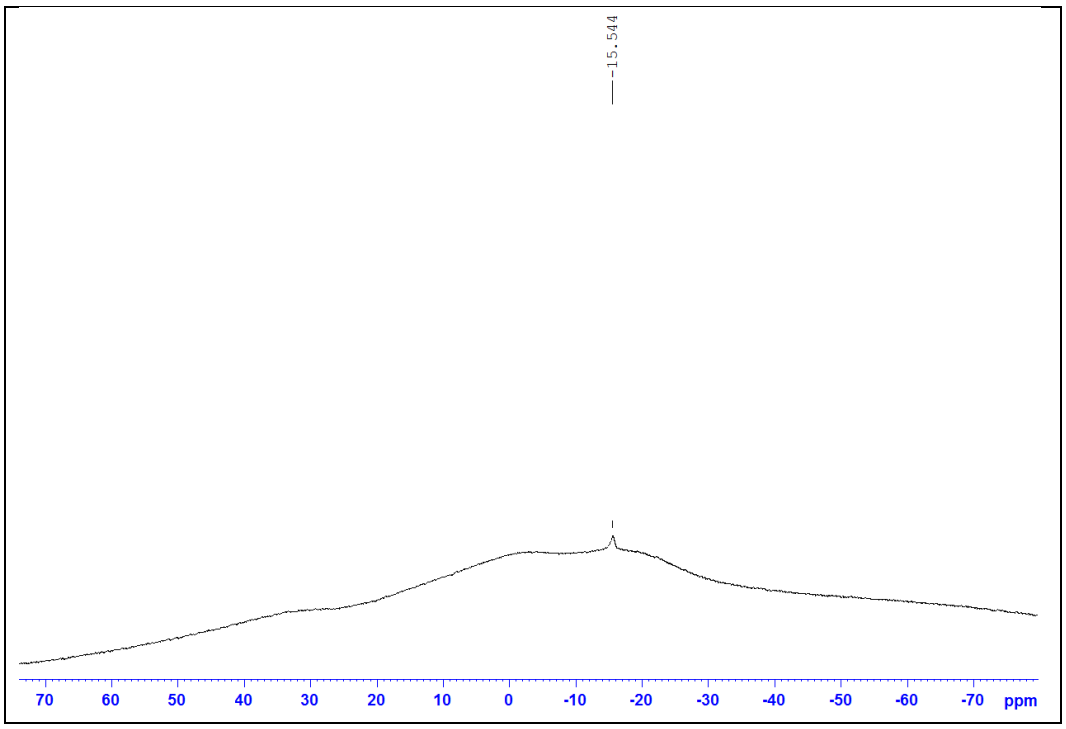
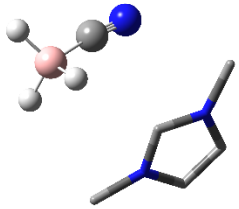


Figure S14. ^{11}B NMR spectrum of $[Cs^+]_2[B_{12}I_{12}^{2-}]$ promoter **2**. (*top*): immediately upon addition of H_2O_2 (30%); (*bottom*): after 10 min. after addition of H_2O_2 (30%).

^{1}H NMR (DMSO-d_6) of the reaction products showed a disappearance of H_2O_2 peak at 10.4 ppm.

DFT Calculations

DFT calculations were performed using Gaussian 09.2 Geometry optimization of all the molecules, intermediates were carried out using the wB97XD method with Ahlrichs' def2-SVP basis set, and with the relativistic effect of iodine, which was accounted for by the Stuttgart-Dresden ECP, implemented in the Gaussian 09 software. Thermal energy corrections were extracted from the results of frequency analysis performed at the same level of theory. Frequency analysis of all the molecules and intermediates contained no imaginary frequency showing that these are energy minima.



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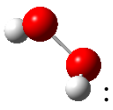

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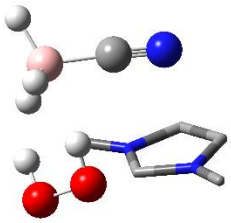

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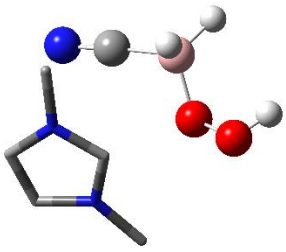

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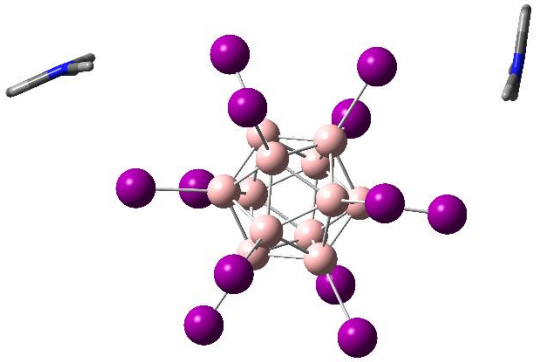

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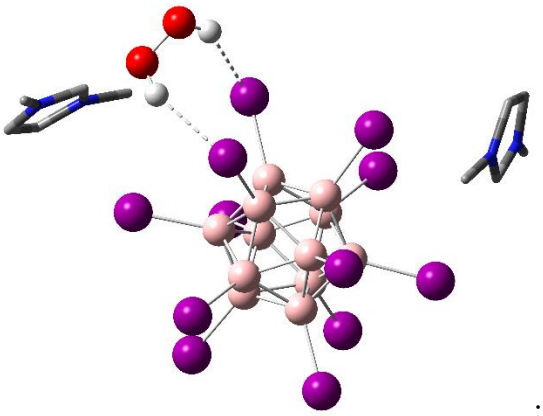

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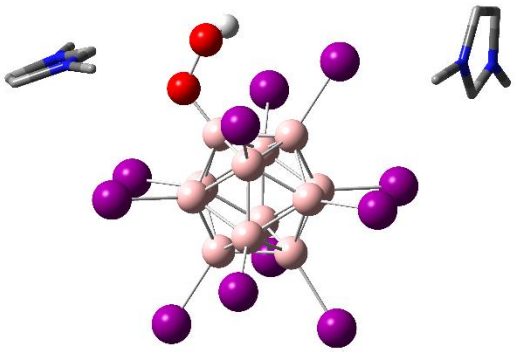

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B	-1.70619100	0.31632800	0.48092500
I	-0.10100300	3.21975400	1.62107900
B	-0.17623000	1.20412700	0.73857000
I	1.12153900	-3.31482500	2.15507200
B	0.37018300	-1.65284400	0.95733100
I	-2.88608300	-2.83450900	1.35905400
B	-1.38416900	-1.44415700	0.60927800
I	-0.95640800	-0.17026900	3.83912500
B	-0.53878200	-0.28090300	1.69888000
I	2.77801200	0.37608900	2.41348700
B	1.10545700	-0.01239700	1.03475900
I	3.22181500	-1.86861500	-1.03961300
B	1.29048600	-1.00912400	-0.44925400

I	-0.28831200	-3.85521200	-1.68016600
B	-0.24526600	-1.89750000	-0.72083300
O	-1.44601000	1.93007500	-1.75912900
O	-0.65721100	3.06109900	-2.07599700
H	-0.12141100	2.74601600	-2.82267000
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C	-5.40777700	4.25170200	-0.41277400
C	-5.57781900	3.50571800	-1.53847500
N	-4.34033500	3.36379000	-2.11957100
H	-2.36795600	4.02604100	-1.56621900
H	-6.11990400	4.57305200	0.34090500
H	-6.46879100	3.05297400	-1.96228600
N	-4.06791500	4.55666700	-0.33356400
C	-3.41798900	5.22312500	0.78457700
H	-4.03536800	6.06960800	1.10835500
H	-3.28165200	4.50492500	1.60550800
H	-2.43445400	5.58424400	0.46454400
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H	-4.05070100	3.31806100	-4.20354300
H	-3.07142800	2.14086800	-3.23282800
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C	6.51147000	2.64914700	-1.51927400
C	6.10933800	3.55801200	-0.58877200
C	5.56734500	1.55541400	0.13924400
N	6.17513800	1.40603200	-1.03686800
H	7.00979900	2.78278100	-2.47455900
H	6.18993800	4.64066200	-0.57391400
H	5.11555800	0.75817700	0.73355500
N	5.53682200	2.85358100	0.44414600
C	4.87062400	3.44446600	1.59998300
H	5.04392900	2.82271500	2.48460000
H	5.29105200	4.44239400	1.76756300
H	3.78959700	3.50983900	1.40925400
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H	6.30495200	-0.67933100	-1.03697500
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H	7.32555400	0.15427500	-2.25057200

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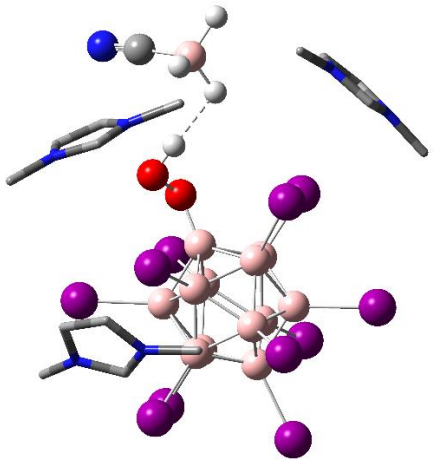
Sum of electronic and thermal Free Energies= -1185.103755



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I	-1.44538000	3.10091800	0.00877400
B	-0.46894400	1.16542000	-0.31849100
I	-3.47997700	-0.20110500	-1.41269200
B	-1.34203100	-0.27082200	-0.91921700
I	-1.83795400	-3.47800200	0.36424000
B	-0.63018700	-1.72103200	-0.13891600
I	1.18537200	-2.19324600	2.81840100
B	0.68807600	-1.17167300	0.93763300
I	2.82727500	-0.65607000	-3.44872900
B	1.40885100	-0.48174800	-1.80105900
I	-0.83601600	-2.51553600	-3.52609000
B	-0.19761700	-1.29897100	-1.83343300
I	2.05206400	-3.79894100	-0.89001000
B	1.07282700	-1.86000700	-0.68375100
I	4.08869500	-0.56260300	0.37669600
B	1.94174000	-0.41232100	-0.08428800
I	2.43483000	2.82234200	-1.31417000
B	1.23134300	1.04292000	-0.85411500
I	-0.60076500	1.59142600	-3.77247200
B	-0.09035800	0.49957600	-1.94093500
O	-1.89753900	-0.20476300	1.73944600
O	-1.67477500	0.57399200	2.90189200
H	-2.38459100	1.24535800	2.82254500
C	-3.08492800	-2.05495500	3.72642500
C	-3.58430900	-4.16932100	4.10253500
C	-4.49135600	-3.66868600	3.22260700
N	-4.15952300	-2.35263200	3.00416300
H	-2.58854100	-1.08288300	3.75641300
H	-3.47624800	-5.16120100	4.52974300
H	-5.33684600	-4.13802200	2.72977900
C	-4.37950700	4.57421800	-0.81496600
C	-5.65617900	3.19410600	0.32197000
C	-5.60926600	2.76550100	-0.96968300
N	-4.80702100	3.64187000	-1.66363200
H	-3.70959800	5.39186200	-1.06761900
H	-6.11363500	2.76978800	1.21223200
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N	-2.71841500	-3.14073800	4.40678700
N	-4.88701500	4.33183800	0.39127100
C	-1.57602400	-3.23542500	5.29679700
H	-1.89124900	-3.67818200	6.25003600
H	-0.79224700	-3.84842900	4.83277300
H	-1.18206200	-2.22904900	5.47529800
C	-4.87886000	-1.43217100	2.13896900
H	-5.77537200	-1.07047400	2.65809900
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H	-5.51004300	5.48602000	2.02950500
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H	-3.89228700	5.88662600	1.36345500
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H	-3.92131600	4.40899700	-3.39610600
H	-3.53442700	2.69627700	-3.03574000

H	-5.15922100	3.14503900	-3.66694400
H	-3.66952100	2.97271600	3.93830400
H	-4.05929500	1.75339200	2.37038200
H	-5.57412400	2.69619000	3.30745700
C	-4.61552700	0.92252800	4.44486800
N	-4.69559000	-0.02643900	5.11253600
B	-4.47140100	2.16441000	3.46687600
C	4.41852800	3.99588300	4.02483300
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C	4.76257300	2.41095100	2.54018400
N	4.56488400	3.71981700	2.68481300
H	4.23143700	5.00009100	4.39261400
H	4.51733700	2.59222600	5.75164300
H	4.83586300	1.87489700	1.59194500
N	4.79003800	1.84307700	3.74562600
C	4.86437100	0.40884900	4.00436700
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H	5.17037400	0.25944900	5.04574700
H	3.87976400	-0.04845900	3.82469100
C	4.35796400	4.66242400	1.59431500
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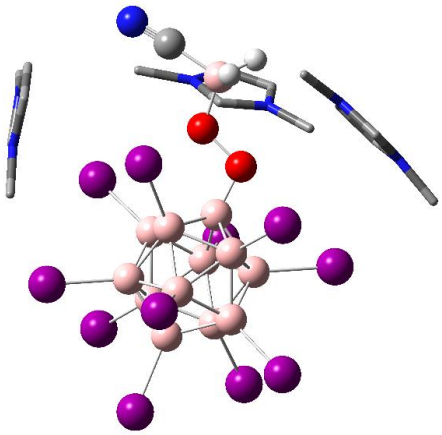

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I	-0.55125300	1.42352700	-3.37671500
B	-0.64456900	0.52662700	-1.37123500
I	-1.62591000	3.60125300	-0.00850500
B	-1.13145600	1.45329600	0.07749400
I	0.28196800	1.98698000	3.23065500
B	-0.29135900	0.76421900	1.49676000
I	2.58755100	-1.15910100	1.97949400
B	0.74517900	-0.57010000	0.92000400
I	-3.67942100	-2.69405900	0.70601800
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I	-0.98595600	-1.86615700	3.67237300
B	-0.84355000	-0.92782400	1.70409600
I	0.17019700	-3.97953800	0.38610700
B	-0.32654700	-1.84013400	0.24321400
I	-1.71789600	-2.41753100	-2.89645200
B	-1.18445900	-1.16834600	-1.17723800
I	-4.10676700	0.70038100	-1.59133900
B	-2.22298500	0.19190800	-0.60389400
O	1.56755600	1.90567000	-0.36910800
O	2.84731900	1.34593500	-0.08469000
C	3.61603700	2.83891400	2.22324400
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N	4.48878600	2.66940300	3.21487300
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C	5.19475900	1.42466600	3.48926100
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C	2.94278600	2.92356900	-4.55457500
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H	-1.81914400	4.78166800	-3.17263900
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H	2.05558900	-5.84102600	-1.73090100

H	1.63347100	-4.39426000	-2.69715100
H	2.64182300	-5.70504900	-3.41563300
H	3.77436800	1.81803500	-2.11111500
H	4.11798000	3.15586100	-0.61704100
C	5.19935900	1.11312700	-0.41384000
N	6.08481600	0.47742900	-0.01228900
B	3.92509500	1.95643300	-0.90191700

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References

1. M. A. Juhasz, G. R. Matheson, P. S. Chang, A. Rosenbaum, D. H. Juers, *Synth. React. Inorg. Met.-Org. Nano-Met. Chem.,* 2016, **46**, 583-588.
2. (a) J. K. Lindsay, C. R. Hauser, *J. Org. Chem*., 1957, **22**, 355-358; (b) P. J. Graham, R. V. Lindsey, G. W. Parshall, M. L. Peterson, G. M. Whitman, *J. Am. Chem. Soc*., 1957, **79**, 3416-3420.
3. (a) W. C. Bray, H. A. Liebhafsky, *J. Am. Chem. Soc*., 1931, **53**, 38-44; (b) K. J. Morgan, *Quat. Rev*., 1954, **8**, 123-146.