Supplementary Material

o-Carboranylalkoxy-1,3,5-Triazine Derivatives: Synthesis, Characterization, Cytotoxicity, and X-ray Structural Studies

1.	Bond lengths, angles, and torsion angles of compound **5**.	S2
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3.	Bond lengths, angles, and torsion angles of compound **6**.	S23
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Table S1. Bond lengths (Å) of **3**.

Al1–C1	1.938(12)	B3–B4	1.767(14)
Al1–N1	2.039(10)	B3–B8	1.779(15)
Al1–Br1	2.216(2)	B3–B7	1.781(15)
Al1–Br#1	2.216(2)	B4–B8	1.771(14)
N1–C14	1.476(10)	B4–B9	1.792(15)
N1–C#14	1.476(10)	B4–B#4	1.80(2)
N1–C13	1.518(17)	B7–B#7	1.73(2)
C1–C2	1.649(15)	B7–B8	1.774(16)
C1–B3	1.712(11)	B7–B12	1.780(19)
C1–B#3	1.712(11)	B8–B9	1.784(14)
C1–B4	1.736(13)	B8–B12	1.793(15)
C1–B#4	1.736(13)	B9–B8	1.784(14)
C2–C13	1.516(17)	B9–B4	1.792(15)
C2–B7	1.683(13)	B9–B12	1.81(2)
C2–B#7	1.683(13)	B12–B7	1.780(19)
C2–B3	1.685(11)	B12–B8	1.793(15)
C2–B#3	1.686(11)		

Table S2. Bond angles (º) of **3**.

C1 Al1 N1	92.2(4)	C1 C2 B#7	113.4(7)
C1 Al1 Br1	113.65(15)	C13 C2 B7	121.6(8)
N1 Al1 Br1	109.54(16)	C1 C2 B7	113.4(7)
C1 Al1 Br1	113.65(15)	B7 C2 B#7	61.8(9)
N1 Al1 Br1	109.54(16)	C13 C2 B3	115.6(6)
Br1 Al1 Br1	115.65(16)	C1 C2 B3	61.8(5)
C14 N1 C#14	108.6(12)	B7 C2 B#3	115.1(9)
C14 N1 C13	109.2(8)	B7 C2 B3	63.9(6)
C#14 N1 C13	109.2(8)	C13 C2 B#3	115.6(6)
C#14 N1 Al1	110.1(6)	C1 C2 B#3	61.8(5)
C14 N1 Al1	110.1(6)	B#7 C2 B3	63.9(6)
C13 N1 Al1	109.4(8)	B7 C2 B#3	115.1(9)
C2 C1 B3	60.2(5)	B3 C2 B#3	114.8(10)
C2 C1 B#3	60.2(5)	C2 C13 N1	115.6(11)
B3 C1 B#3	112.1(9)	C2 B3 C1	58.1(5)
C2 C1 B4	108.5(7)	C2 B3 B4	105.4(7)
B3 C1 B4	61.7(5)	C1 B3 B4	59.8(6)
B3 C1 B#4	112.8(8)	C2 B3 B8	104.2(8)
C2 C1 B#4	108.5(7)	C1 B3 B8	106.1(8)
B3 C1 B#4	112.8(8)	B4 B3 B8	59.9(6)
B3 C1 B4	61.7(5)	C2 B3 B7	58.0(6)
B4 C1 B#4	62.6(8)	C1 B3 B7	105.7(7)
C2 C1 Al1	107.9(7)	B4 B3 B7	107.9(8)
B3 C1 Al1	113.2(5)	B8 B3 B7	59.8(6)
B#3 C1 Al1	113.2(5)	C1 B4 B3	58.5(5)
B4 C1 Al1	131.1(6)	C1 B4 B8	105.5(7)
B#4 C1 Al1	131.1(6)	B3 B4 B8	60.4(6)
C13 C2 C1	114.8(9)	C1 B4 B9	105.6(7)
C13 C2 B7	121.6(8)	B3 B4 B9	108.3(8)
B8 B4 B9	60.1(6)	C1 B4 B#4	58.7(4)
B8 B4 B#4	107.5(6)	B3 B4 B#4	107.0(4)
B9 B4 B#4	59.8(4)	C2 B7 B#7	59.1(5)
C2 B7 B8	104.6(7)	B#7 B7 B8	108.7(5)
C2 B7 B12	106.2(8)	B#7 B7 B12	61.0(4)
B8 B7 B12	60.6(7)	C2 B7 B3	58.1(5)
B#7 B7 B3	108.2(5)	B8 B7 B3	60.1(6)
B12 B7 B3	109.2(8)	B4 B8 B7	108.1(8)
B4 B8 B3	59.7(6)	B7 B8 B3	60.2(6)
B4 B8 B9	60.5(7)	B7 B8 B9	107.9(9)
B3 B8 B9	108.1(8)	B4 B8 B12	109.5(8)
B7 B8 B12	59.9(8)	B3 B8 B12	108.7(8)
B9 B8 B12	60.7(8)	B8 B9 B#8	106.8(12)
B#8 B9 B4	107.4(9)	B8 B9 B4	59.4(5)
B#8 B9 B#4	59.4(5)	B#8 B9 B4	107.4(9)
B4 B9 B#4	60.5(8)	B#8 B9 B12	59.9(7)
B8 B9 B12	59.9(7)	B4 B9 B12	108.0(8)
B#4 B9 B12	108.0(8)	B7 B12 B#7	58.1(9)

B#7 B12 B#8	59.5(6)	B#7 B12 B8	105.6(9)
B7 B12 B#8	105.6(9)	B7 B12 B8	59.5(6)
B8 B12 B#8	106.1(10)	B#7 B12 B9	106.6(8)
B7 B12 B9	106.6(8)	B#8 B12 B9	59.4(6)
B8 B12 B9	59.4(6)		

Table S3. Torsional angles (º) of **3**.

C1 Al1 N1 C#14	-120.1(7)	Br#1 Al1 N1 C#14	-4.0(8)
Br1 Al1 N1 C#14	123.8(7)	C1 Al1 N1 C14	120.1(7)
Br#1 Al1 N1 C14	-123.8(7)	Br1 Al1 N1 C14	4.0(8)
C1 Al1 N1 C13	0.000(1)	Br#1 Al1 N1 C13	116.09(14)
Br1 Al1 N1 C13	-116.09(14)	N1 Al1 C1 C2	0.000(1)
Br#1 Al1 C1 C2	-112.47(18)	Br1 Al1 C1 C2	112.47(18)
N1 Al1 C1 B3	-64.5(6)	Br#1 Al1 C1 B3	-177.0(5)
Br1 Al1 C1 B3	48.0(7)	N1 Al1 C1 B#3	64.5(6)
Br#1 Al1 C1 B#3	-48.0(7)	Br1 Al1 C1 B#3	177.0(5)
N1 Al1 C1 B4	-136.4(7)	Br#1 Al1 C1 B4	111.1(6)
Br1 Al1 C1 B4	-23.9(8)	N1 Al1 C1 B#4	136.4(7)
Br#1 Al1 C1 B#4	23.9(8)	Br1 Al1 C1 B#4	-111.1(6)
B3 C1 C2 C13	107.0(5)	B#3 C1 C2 C13	-107.0(5)
B4 C1 C2 C13	146.8(5)	B#4 C1 C2 C13	-146.8(5)
Al1 C1 C2 C13	0.000(2)	B3 C1 C2 B#7	-107.0(9)
B#3 C1 C2 B#7	39.0(7)	B4 C1 C2 B#7	-67.2(7)
B#4 C1 C2 B#7	-0.8(8)	Al1 C1 C2 B7	146.0(6)
B3 C1 C2 B7	-39.0(7)	B#3 C1 C2 B7	107.0(9)
B4 C1 C2 B7	0.8(8)	B#4 C1 C2 B7	67.2(7)
Al1 C1 C2 B7	-146.0(6)	B#3 C1 C2 B3	146.0(10)
B4 C1 C2 B3	39.8(6)	B#4 C1 C2 B3	106.2(8)
Al1 C1 C2 B3	-107.0(5)	B3 C1 C2 B#3	-146.0(10)
B4 C1 C2 B#3	-106.2(8)	B#4 C1 C2 B#3	-39.8(6)
Al1 C1 C2 B#3	107.0(5)	C1 C2 C13 N1	0.000(3)
B#7 C2 C13 N1	-142.9(6)	B7 C2 C13 N1	142.9(6)
B3 C2 C13 N1	69.1(7)	B#3 C2 C13 N1	-69.1(7)
C#14 N1 C13 C2	120.7(7)	C14 N1 C13 C2	-120.7(7)
Al1 N1 C13 C2	0.000(2)	C13 C2 B3 C1	-105.7(10)
B#7 C2 B3 C1	104.2(8)	B7 C2 B3 C1	140.0(8)
B#3 C2 B3 C1	32.9(9)	C13 C2 B3 B4	-143.9(9)
C1 C2 B3 B4	-38.2(7)	B#7 C2 B3 B4	66.0(9)
B7 C2 B3 B4	101.7(8)	B#3 C2 B3 B4	-5.4(13)
C13 C2 B3 B8	153.9(9)	C1 C2 B3 B8	-100.4(8)
B#7 C2 B3 B8	3.9(10)	B7 C2 B3 B8	39.6(7)
B#3 C2 B3 B8	-67.5(11)	C13 C2 B3 B7	114.3(10)
C1 C2 B3 B7	-140.0(8)	B#7 C2 B3 B7	-35.7(7)
B#3 C2 B3 B7	-107.1(10)	B#3 C1 B3 C2	-31.5(9)
B4 C1 B3 C2	-136.4(8)	B#4 C1 B3 C2	-98.9(8)
Al1 C1 B3 C2	98.0(7)	C2 C1 B3 B4	136.4(8)
B#3 C1 B3 B4	104.8(9)	B#4 C1 B3 B4	37.5(7)
Al1 C1 B3 B4	-125.6(7)	C2 C1 B3 B8	96.9(8)
B#3 C1 B3 B8	65.4(11)	B4 C1 B3 B8	-39.5(7)
B#4 C1 B3 B8	-2.0(9)	Al1 C1 B3 B8	-165.0(7)
C2 C1 B3 B7	34.5(7)	B#3 C1 B3 B7	3.0(12)
B4 C1 B3 B7	-101.9(8)	B#4 C1 B3 B7	-64.4(9)
Al1 C1 B3 B7	132.6(6)	C2 C1 B4 B3	-39.1(6)
B#3 C1 B4 B3	-103.7(10)	B#4 C1 B4 B3	-140.8(6)

Al1 C1 B4 B3	97.1(7)
B3 C1 B4 B8	39.5(7)
B#4 C1 B4 B8	-101.3(7)
C2 C1 B4 B9	63.1(8)
B#3 C1 B4 B9	-1.6(9)
Al1 C1 B4 B9	-160.7(6)
B3 C1 B4 B#4	140.8(6)
Al1 C1 B4 B#4	-122.1(8)
B8 B3 B4 C1	135.1(8)
C2 B3 B4 B8	-97.7(8)
B7 B3 B4 B8	-37.0(7)
C1 B3 B4 B9	-97.4(7)
B7 B3 B4 B9	0.7(9)
C1 B3 B4 B#4	-34.4(5)
B7 B3 B4 B#4	63.7(6)
C1 C2 B7 B#7	-105.0(6)
B#3 C2 B7 B#7	-36.5(5)
C1 C2 B7 B8	-1.6(9)
B3 C2 B7 B8	-39.8(7)
C13 C2 B7 B12	151.9(8)
B#7 C2 B7 B12	40.3(8)
B#3 C2 B7 B12	3.8(10)
C1 C2 B7 B3	38.1(6)
B#3 C2 B7 B3	106.7(10)
B4 B3 B7 C2	-97.3(7)
C2 B3 B7 B#7	32.8(5)
B4 B3 B7 B#7	-64.5(6)
C2 B3 B7 B8	134.4(8)
B4 B3 B7 B8	37.1(7)
C1 B3 B7 B12	63.0(9)
B8 B3 B7 B12	-36.8(7)
B3 B4 B8 B7	37.2(7)
B#4 B4 B8 B7	-62.8(7)
B9 B4 B8 B3	-137.9(8)
C1 B4 B8 B9	99.3(8)
B#4 B4 B8 B9	37.9(6)
B3 B4 B8 B12	100.8(9)
B#4 B4 B8 B12	0.7(9)
B#7 B7 B8 B4	63.7(8)
B3 B7 B8 B4	-37.0(8)
B#7 B7 B8 B3	100.7(5)
C2 B7 B8 B9	-62.2(10)
B12 B7 B8 B9	38.5(9)
C2 B7 B8 B12	-100.7(8)
B3 B7 B8 B12	-139.5(8)
C1 B3 B8 B4	39.4(7)
C2 B3 B8 B7	-38.7(7)
B4 B3 B8 B7	-138.5(8)
C1 B3 B8 B9	1.6(11)
C2 C1 B4 B8	0.4(8)
B#3 C1 B4 B8	-64.2(9)
Al1 C1 B4 B8	136.7(7)
B3 C1 B4 B9	102.2(8)
B#4 C1 B4 B9	-38.7(8)
C2 C1 B4 B#4	101.7(6)
B#3 C1 B4 B#4	37.1(5)
C2 B3 B4 C1	37.4(7)
B7 B3 B4 C1	98.1(8)
C1 B3 B4 B8	-135.1(8)
C2 B3 B4 B9	-60.0(8)
B8 B3 B4 B9	37.7(6)
C2 B3 B4 B#4	3.0(7)
B8 B3 B4 B#4	100.7(6)
C13 C2 B7 B#7	111.6(8)
B3 C2 B7 B#7	-143.1(6)
C13 C2 B7 B8	-145.0(8)
B#7 C2 B7 B8	103.4(6)
B#3 C2 B7 B8	66.9(9)
C1 C2 B7 B12	-64.7(8)
B3 C2 B7 B12	-102.9(8)
C13 C2 B7 B3	-105.3(8)
B#7 C2 B7 B3	143.1(6)
C1 B3 B7 C2	-34.6(7)
B8 B3 B7 C2	-134.4(8)
C1 B3 B7 B#7	-1.7(7)
B8 B3 B7 B#7	-101.6(5)
C1 B3 B7 B8	99.8(8)
C2 B3 B7 B12	97.6(8)
B4 B3 B7 B12	0.3(9)
C1 B4 B8 B7	-1.4(10)
B9 B4 B8 B7	-100.7(9)
C1 B4 B8 B3	-38.6(6)
B#4 B4 B8 B3	-100.1(5)
B3 B4 B8 B9	137.9(8)
C1 B4 B8 B12	62.2(9)
B9 B4 B8 B12	-37.1(8)
C2 B7 B8 B4	1.8(10)
B12 B7 B8 B4	102.5(9)
C2 B7 B8 B3	38.8(6)
B12 B7 B8 B3	139.5(8)
B#7 B7 B8 B9	-0.3(9)
B3 B7 B8 B9	-101.0(9)
B#7 B7 B8 B12	-38.8(5)
C2 B3 B8 B4	99.8(8)
B7 B3 B8 B4	138.5(8)
C1 B3 B8 B7	-99.0(8)
C2 B3 B8 B9	62.0(10)
B4 B3 B8 B9	-37.8(8)

B7 B3 B8 B9	100.6(10)	C2 B3 B8 B12	-2.3(10)
C1 B3 B8 B12	-62.7(9)	B4 B3 B8 B12	-102.1(9)
B7 B3 B8 B12	36.4(8)	B4 B8 B9 B#8	-100.6(10)
B7 B8 B9 B#8	0.5(14)	B3 B8 B9 B#8	-63.1(13)
B12 B8 B9 B#8	38.7(10)	B7 B8 B9 B4	101.1(8)
B3 B8 B9 B4	37.5(7)	B12 B8 B9 B4	139.2(9)
B4 B8 B9 B#4	-38.2(8)	B7 B8 B9 B#4	62.9(11)
B3 B8 B9 B#4	-0.7(12)	B12 B8 B9 B#4	101.1(9)
B4 B8 B9 B12	-139.2(9)	B7 B8 B9 B12	-38.2(8)
B3 B8 B9 B12	-101.8(9)	C1 B4 B9 B#8	0.5(11)
B3 B4 B9 B#8	61.8(10)	B8 B4 B9 B#8	99.6(12)
B#4 B4 B9 B#8	-37.7(6)	C1 B4 B9 B8	-99.2(8)
B3 B4 B9 B8	-37.8(7)	B#4 B4 B9 B8	-137.3(7)
C1 B4 B9 B#4	38.1(7)	B3 B4 B9 B#4	99.5(6)
B8 B4 B9 B#4	137.3(7)	C1 B4 B9 B12	-62.7(8)
B3 B4 B9 B12	-1.4(8)	B8 B4 B9 B12	36.4(7)
B#4 B4 B9 B12	-100.9(6)	C2 B7 B12 B#7	-39.4(8)
B8 B7 B12 B7	-137.2(6)	B3 B7 B12 B#7	-100.7(7)
C2 B7 B12 B#8	-2.0(10)	B#7 B7 B12 B#8	37.4(5)
B8 B7 B12 B#8	-99.8(10)	B3 B7 B12 B8	-63.2(9)
C2 B7 B12 B8	97.8(8)	B7 B7 B12 B8	137.2(6)
B3 B7 B12 B8	36.6(7)	C2 B7 B12 B9	60.2(8)
B#7 B7 B12 B9	99.6(6)	B8 B7 B12 B9	-37.7(6)
B3 B7 B12 B9	-1.1(8)	B4 B8 B12 B#7	-63.3(10)
B7 B8 B12 B#7	36.8(7)	B3 B8 B12 B#7	0.3(10)
B9 B8 B12 B#7	-100.4(8)	B4 B8 B12 B7	-100.1(8)
B3 B8 B12 B7	-36.5(7)	B9 B8 B12 B7	-137.2(9)
B4 B8 B12 B#8	-1.2(14)	B7 B8 B12 B#8	98.9(10)
B3 B8 B12 B#8	62.4(12)	B9 B8 B12 B#8	-38.3(10)
B4 B8 B12 B9	37.1(8)	B7 B8 B12 B9	137.2(9)
B3 B8 B12 B9	100.7(9)	B#8 B9 B12 B#7	-37.7(7)
B8 B9 B12 B#7	98.6(8)	B4 B9 B12 B#7	62.4(6)
B#4 B9 B12 B#7	-1.5(8)	B#8 B9 B12 B7	-98.6(8)
B8 B9 B12 B7	37.7(7)	B4 B9 B12 B7	1.5(8)
B#4 B9 B12 B7	-62.4(6)	B8 B9 B12 B#8	136.3(11)
B4 B9 B12 B#8	100.1(8)	B#4 B9 B12 B#8	36.2(6)
B#8 B9 B12 B8	-136.3(11)	B4 B9 B12 B8	-36.2(6)
B#4 B9 B12 B8	-100.1(8)		

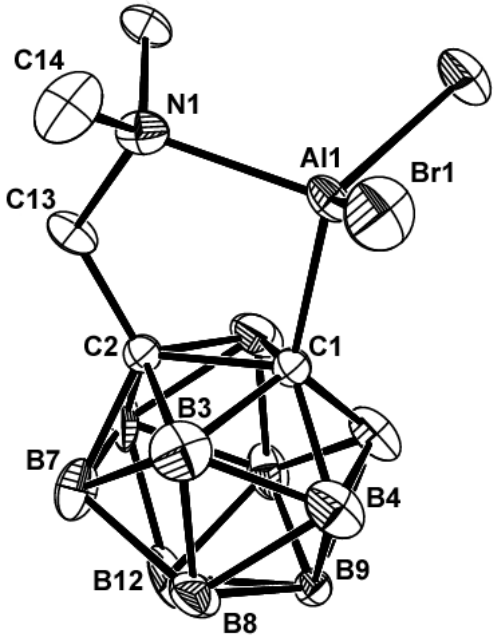

Figure S1. Molecular structure of **3**.

Table S4. Bond lengths (Å) of **4**.

Al1 C#15	1.947(5)	N1 C#14	1.488(5)
Al1 C15	1.947(5)	N1 C14	1.488(5)
Al1 C1	2.010(6)	N1 C13	1.507(7)
Al1 N1	2.090(5)	C1 C2	1.652(8)
C1 B4	1.701(6)	C1 B#4	1.701(6)
C1 B3	1.717(6)	C1 B#3	1.717(6)
C2 C13	1.532(8)	C2 B7	1.688(6)
C2 B3	1.690(5)	C2 B#7	1.688(6)
C2 B#3	1.690(5)	B3 B7	1.755(7)
B3 B4	1.761(7)	B3 B8	1.774(7)
B4 B#4	1.745(9)	B4 B9	1.780(8)
B4 B8	1.781(8)	B7 B12	1.772(9)
B7 B#7	1.777(11)	B7 B8	1.786(8)
B8 B9	1.766(7)	B8 B12	1.788(7)
B9 B12	1.761(11)	B#9 B8	1.766(7)
B#9 B4	1.780(8)	B12 B#7	1.772(9)
B12 B#8	1.788(7)		

Table S5. Bond angles (º) of **4**.

C#15 Al1 C15	119.4(3)	C#15 Al1 C1	113.11(18)
C15 Al1 C1	113.11(18)	C#15 Al1 N1	109.13(17)
C15 Al1 N1	109.13(17)	C1 Al1 N1	88.4(2)
C#14 N1 C14	108.0(6)	C#14 N1 C13	108.3(3)
C14 N1 C13	108.3(3)	C#14 N1 Al1	109.5(3)
C14 N1 Al1	109.5(3)	C13 N1 Al1	113.2(3)
C2 C1 B4	108.9(4)	C2 C1 B#4	108.9(4)
B4 C1 B#4	61.7(4)	C2 C1 B3	60.2(2)
B4 C1 B3	62.0(3)	B#4 C1 B3	112.3(4)
C2 C1 B#3	60.2(2)	B4 C1 B#3	112.3(4)
B#4 C1 B#3	62.0(3)	B3 C1 B#3	111.7(5)
C2 C1 Al1	108.9(3)	B4 C1 Al1	130.3(3)
B#4 C1 Al1	130.3(3)	B3 C1 Al1	114.0(2)
C13 C2 C1	115.9(5)	B#3 C1 Al1	114.0(2)
C13 C2 B7	120.8(4)	C1 C2 B7	112.8(4)
C13 C2 B#7	120.8(4)	C1 C2 B7	112.8(4)
B7 C2 B#7	63.5(4)	C13 C2 B3	116.3(3)
C1 C2 B3	61.8(2)	B7 C2 B3	62.6(3)
B#7 C2 B3	115.2(4)	C13 C2 B#3	116.3(3)
C1 C2 B#3	61.8(2)	B7 C2 B#3	115.2(4)
B#7 C2 B#3	62.6(3)	B3 C2 B#3	114.5(4)
N1 C13 C2	113.6(5)	C2 B3 C1	58.0(3)
C2 B3 B7	58.6(3)	C1 B3 B7	106.4(4)
C2 B3 B4	104.5(3)	C1 B3 B4	58.5(3)
B7 B3 B4	108.8(4)	C2 B3 B8	105.4(4)
C1 B3 B8	106.4(4)	B7 B3 B8	60.8(3)
B4 B3 B8	60.5(3)	C1 B4 B#4	59.13(19)
C1 B4 B3	59.5(3)	B#4 B4 B3	108.2(2)
C1 B4 B9	106.0(4)	B#4 B4 B9	60.6(2)
B3 B4 B9	107.1(4)	C1 B4 B8	106.8(4)
B#4 B4 B8	108.8(3)	B3 B4 B8	60.1(3)
B9 B4 B8	59.4(3)	C2 B7 B3	58.7(3)
C2 B7 B12	104.4(4)	B3 B7 B12	108.1(4)
C2 B7 B#7	58.2(2)	B3 B7 B#7	107.7(2)
B12 B7 B#7	59.9(2)	C2 B7 B8	104.9(4)
B3 B7 B8	60.1(3)	B12 B7 B8	60.3(3)
B#7 B7 B8	108.2(3)	B9 B8 B3	107.2(4)
B9 B8 B4	60.3(3)	B3 B8 B4	59.4(3)
B9 B8 B7	106.8(4)	B3 B8 B7	59.1(3)
B4 B8 B7	106.5(4)	B3 B8 B12	106.6(4)
B9 B8 B12	59.4(4)	B4 B8 B12	107.2(4)
B7 B8 B12	59.5(3)	B12 B9 B#8	60.9(3)
B12 B9 B8	60.9(3)	B#8 B9 B8	110.0(6)
B12 B9 B#4	108.4(4)	B#8 B9 B#4	60.3(3)
B8 B9 B#4	107.9(5)	B12 B9 B4	108.4(4)
B#8 B9 B4	107.9(5)	B8 B9 B4	60.3(3)
B#4 B9 B4	58.7(4)	B9 B12 B#7	107.6(5)
B9 B12 B7	107.6(5)	B#7 B12 B7	60.2(4)
B9 B12 B8	59.7(3)	B#7 B12 B8	108.3(4)
B7 B12 B8	60.2(3)	B9 B12 B#8	59.7(3)
B#7 B12 B#8	60.2(3)	B7 B12 B#8	108.3(4)
B8 B12 B#8	108.0(5)		

Table S6. Torsional angles (º) of **4**.

B4 B8 B12 B#8	-1.8(6)	B7 B8 B12 B#8	-101.2(5)
B9 B8 B12 B#8	36.3(5)	B3 B8 B12 B#8	-64.2(5)
B3 B8 B12 B7	37.0(4)	B4 B8 B12 B7	99.4(4)
B7 B8 B12 B#7	-37.5(3)	B9 B8 B12 B7	137.6(5)
B3 B8 B12 B#7	-0.5(5)	B4 B8 B12 B#7	61.9(5)
B7 B8 B12 B9	-137.6(5)	B9 B8 B12 B#7	100.1(5)
B3 B8 B12 B9	-100.5(4)	B4 B8 B12 B9	-38.2(4)
B#7 B7 B12 B#8	-37.5(2)	B8 B7 B12 B#8	100.7(5)
C2 B7 B12 B#8	1.5(5)	B3 B7 B12 B#8	62.9(4)
B3 B7 B12 B8	-37.9(4)	B#7 B7 B12 B8	-138.2(3)
B8 B7 B12 B#7	138.2(3)	C2 B7 B12 B8	-99.2(4)
C2 B7 B12 B#7	39.0(4)	B3 B7 B12 B#7	100.4(3)
B#7 B7 B12 B9	-100.6(3)	B8 B7 B12 B9	37.7(3)
B4 B9 B12 B#8	-100.7(4)	B3 B7 B12 B9	-0.2(4)
B#4 B9 B12 B#8	-38.5(3)	C2 B7 B12 B9	-61.5(4)
B4 B9 B12 B8	38.5(3)	B8 B9 B12 B#8	-139.2(6)
B#8 B9 B12 B8	139.2(6)	B#4 B9 B12 B8	100.7(4)
B#4 B9 B12 B7	62.8(3)	B4 B9 B12 B7	0.6(4)
B#8 B9 B12 B7	101.3(4)	B8 B9 B12 B7	-37.9(3)
B#4 B9 B12 B#7	-0.6(4)	B4 B9 B12 B#7	-62.8(3)
B8 B4 B9 B#4	-139.6(3)	B8 B9 B12 B#7	-101.3(4)
B3 B4 B9 B#4	-101.6(3)	B#8 B9 B12 B#7	37.9(3)
B3 B4 B9 B8	38.0(3)	C1 B4 B9 B#4	-39.3(4)
C1 B4 B9 B8	100.3(4)	B#4 B4 B9 B8	139.6(3)
B3 B4 B9 B#8	-65.3(5)	B8 B4 B9 B#8	-103.3(6)
C1 B4 B9 B#8	-3.0(5)	B#4 B4 B9 B#8	36.3(3)
B3 B4 B9 B12	-0.8(4)	B8 B4 B9 B12	-38.8(3)
C1 B4 B9 B12	61.5(4)	B#4 B4 B9 B12	100.8(3)
B7 B8 B9 B4	-99.8(4)	B12 B8 B9 B4	-137.2(4)
B12 B8 B9 B#4	-101.5(4)	B3 B8 B9 B4	-37.7(3)
B4 B8 B9 B#4	35.6(4)	B7 B8 B9 B#4	-64.2(5)
B12 B8 B9 B#8	-37.4(5)	B3 B8 B9 B#4	-2.1(6)
B4 B8 B9 B#8	99.8(6)	B7 B8 B9 B#8	0.0(8)
B7 B8 B9 B12	37.4(4)	B3 B8 B9 B#8	62.1(7)
B3 B8 B9 B12	99.5(4)	B4 B8 B9 B12	137.2(4)
B3 B7 B8 B12	137.7(4)	B#7 B7 B8 B12	37.4(3)
B#7 B7 B8 B4	-63.2(4)	C2 B7 B8 B12	98.3(4)
B3 B7 B8 B4	37.2(3)	B12 B7 B8 B4	-100.5(5)
B#7 B7 B8 B3	-100.3(3)	C2 B7 B8 B4	-2.2(5)
C2 B7 B8 B3	-39.4(3)	B12 B7 B8 B3	-137.7(4)
B12 B7 B8 B9	-37.3(5)	B#7 B7 B8 B9	0.0(5)
B9 B4 B8 B12	37.8(4)	B3 B7 B8 B9	100.4(5)
B3 B4 B8 B12	-99.5(4)	C2 B7 B8 B9	60.9(5)
C1 B4 B8 B12	-61.3(4)	B#4 B4 B8 B12	1.1(4)
B3 B4 B8 B7	-37.1(3)	B9 B4 B8 B7	100.2(5)
C1 B4 B8 B7	1.2(5)	B#4 B4 B8 B7	63.6(4)
B#4 B4 B8 B3	100.6(3)	B9 B4 B8 B3	137.3(4)

B3 B4 B8 B9	-137.3(4)
C1 B4 B8 B9	-99.0(4)
B7 B3 B8 B12	-37.2(4)
C2 B3 B8 B12	2.2(5)
C1 B3 B8 B7	100.0(4)
B7 B3 B8 B4	-137.7(4)
C2 B3 B8 B4	-98.2(3)
B7 B3 B8 B9	-99.6(4)
C2 B3 B8 B9	-60.1(5)
C1 B3 B7 B8	-99.9(4)
B8 B3 B7 B#7	101.3(3)
C1 B3 B7 B#7	1.3(3)
B8 B3 B7 B12	37.9(4)
C1 B3 B7 B12	-62.0(4)
B8 B3 B7 C2	134.1(4)
C1 B3 B7 C2	34.2(3)
B3 C2 B7 B8	40.1(3)
C1 C2 B7 B8	2.6(4)
B#3 C2 B7 B#7	36.7(2)
C1 C2 B7 B#7	105.1(3)
B#3 C2 B7 B12	-3.2(5)
B#7 C2 B7 B12	-39.9(4)
C13 C2 B7 B12	-151.5(4)
B#7 C2 B7 B3	-142.5(3)
C13 C2 B7 B3	105.9(4)
C1 B3 B4 B8	136.5(4)
B8 B3 B4 B9	-37.7(3)
C1 B3 B4 B9	98.8(4)
B8 B3 B4 B#4	-101.7(3)
C2 B3 B4 B#4	-2.0(4)
B8 B3 B4 C1	-136.5(4)
C2 B3 B4 C1	-36.9(3)
Al1 C1 B4 B8	-137.3(4)
B#4 C1 B4 B8	102.2(3)
Al1 C1 B4 B9	160.4(3)
B3 C1 B4 B9	-100.8(4)
C2 C1 B4 B9	-61.8(3)
B#3 C1 B4 B3	103.6(5)
C2 C1 B4 B3	38.9(3)
B#3 C1 B4 B#4	-37.2(2)
C2 C1 B4 B#4	-101.8(3)
B#3 C1 B3 B8	-65.9(5)
B4 C1 B3 B8	38.6(4)
Al1 C1 B3 B4	124.4(4)
B#4 C1 B3 B4	-37.1(3)
Al1 C1 B3 B7	-133.3(3)
B#4 C1 B3 B7	65.2(4)
C2 C1 B3 B7	-34.5(4)
B#3 C1 B3 C2	32.2(4)
C1 B4 B8 B3	38.2(3)
B#4 B4 B8 B9	-36.7(3)
B4 B3 B8 B12	100.5(4)
C1 B3 B8 B12	62.8(4)
B4 B3 B8 B7	137.7(4)
C2 B3 B8 B7	39.5(3)
C1 B3 B8 B4	-37.7(3)
B4 B3 B8 B9	38.1(4)
C1 B3 B8 B9	0.4(5)
B4 B3 B7 B8	-38.2(3)
C2 B3 B7 B8	-134.1(4)
B4 B3 B7 B#7	63.0(3)
C2 B3 B7 B#7	-32.9(2)
B4 B3 B7 B12	-0.3(5)
C2 B3 B7 B12	-96.2(4)
B4 B3 B7 C2	95.9(4)
B#3 C2 B7 B8	-65.8(5)
B#7 C2 B7 B8	-102.4(3)
C13 C2 B7 B8	145.9(4)
B3 C2 B7 B#7	142.5(3)
C13 C2 B7 B#7	-111.6(4)
B3 C2 B7 B12	102.7(4)
C1 C2 B7 B12	65.2(4)
B#3 C2 B7 B3	-105.9(5)
C1 C2 B7 B3	-37.5(3)
B7 B3 B4 B8	38.4(3)
C2 B3 B4 B8	99.7(4)
B7 B3 B4 B9	0.7(4)
C2 B3 B4 B9	62.0(4)
B7 B3 B4 B#4	-63.3(3)
C1 B3 B4 B#4	34.9(2)
B7 B3 B4 C1	-98.2(4)
B#3 C1 B4 B8	65.1(4)
B3 C1 B4 B8	-38.5(4)
C2 C1 B4 B8	0.4(4)
B#3 C1 B4 B9	2.8(5)
B#4 C1 B4 B9	40.0(4)
Al1 C1 B4 B3	-98.8(3)
B#4 C1 B4 B3	140.7(3)
Al1 C1 B4 B#4	120.4(4)
B3 C1 B4 B#4	-140.7(3)
Al1 C1 B3 B8	163.0(3)
B#4 C1 B3 B8	1.6(5)
C2 C1 B3 B8	-98.2(4)
B#3 C1 B3 B4	-104.6(4)
C2 C1 B3 B4	-136.8(4)
B#3 C1 B3 B7	-2.3(6)
B4 C1 B3 B7	102.3(4)
Al1 C1 B3 C2	-98.8(4)

B4 C1 B3 C2	136.8(4)	B#4 C1 B3 C2	99.7(4)
B#7 C2 B3 B8	-3.5(5)	B#3 C2 B3 B8	66.4(5)
C1 C2 B3 B8	100.0(4)	B7 C2 B3 B8	-40.5(4)
B#3 C2 B3 B4	3.5(6)	C13 C2 B3 B8	-153.2(4)
B7 C2 B3 B4	-103.4(4)	B#7 C2 B3 B4	-66.4(5)
C13 C2 B3 B4	143.9(5)	C1 C2 B3 B4	37.1(4)
B#7 C2 B3 B7	37.0(4)	B#3 C2 B3 B7	106.9(5)
C13 C2 B3 B7	-112.7(5)	C1 C2 B3 B7	140.5(4)
B#3 C2 B3 C1	-33.6(4)	B#7 C2 B3 C1	-103.5(4)
C13 C2 B3 C1	106.8(5)	B7 C2 B3 C1	-140.5(4)
B3 C2 C13 N1	-69.8(4)	B#3 C2 C13 N1	69.8(4)
B7 C2 C13 N1	-142.2(3)	B#7 C2 C13 N1	142.2(3)
Al1 N1 C13 C2	0.0	C1 C2 C13 N1	0.0
C#14 N1 C13 C2	-121.6(3)	C14 N1 C13 C2	121.6(3)
B3 C1 C2 B#3	145.2(5)	Al1 C1 C2 B#3	-107.4(2)
B4 C1 C2 B#3	105.4(4)	B#4 C1 C2 B#3	39.7(3)
B#3 C1 C2 B3	-145.2(5)	Al1 C1 C2 B3	107.4(2)
B4 C1 C2 B3	-39.7(3)	B#4 C1 C2 B3	-105.4(4)
B#3 C1 C2 B#7	-37.8(3)	Al1 C1 C2 B#7	-145.2(3)
B#4 C1 C2 B#7	2.0(4)	B3 C1 C2 B#7	107.4(4)
Al1 C1 C2 B7	145.2(3)	B4 C1 C2 B#7	67.7(3)
B3 C1 C2 B7	37.8(3)	B#3 C1 C2 B7	-107.4(4)
B4 C1 C2 B7	-2.0(4)	B#4 C1 C2 B7 -	67.7(3)
B#3 C1 C2 C13	107.4(2)	Al1 C1 C2 C13	0.0
B#4 C1 C2 C13	147.2(2)	B3 C1 C2 C13	-107.4(2)
N1 Al1 C1 B#3	-65.0(3)	B4 C1 C2 C13	-147.2(2)
C#15 Al1 C1 B#3	45.2(4)	C15 Al1 C1 B#3	-175.1(3)
C15 Al1 C1 B3	-45.2(4)	N1 Al1 C1 B3	65.0(3)
N1 Al1 C1 B#4	-137.7(3)	C#15 Al1 C1 B3	175.1(3)
C#15 Al1 C1 B#4	-27.6(4)	C15 Al1 C1 B#4	112.1(3)
C15 Al1 C1 B4	27.6(4)	N1 Al1 C1 B4	137.7(3)
N1 Al1 C1 C2	0.0	C#15 Al1 C1 B4	-112.1(3)
C#15 Al1 C1 C2	110.15(19)	C15 Al1 C1 C2	-110.15(19)
C15 Al1 N1 C13	113.95(18)	C1 Al1 N1 C13	0.0
C1 Al1 N1 C14	-120.9(3)	C#15 Al1 N1 C13	-113.95(18)
C#15 Al1 N1 C14	125.1(4)	C15 Al1 N1 C14	-7.0(4)
C15 Al1 N1 C#14	-125.1(4)	C1 Al1 N1 C#14	120.9(3)
C#15 Al1 N1 C#14	7.0(4)		

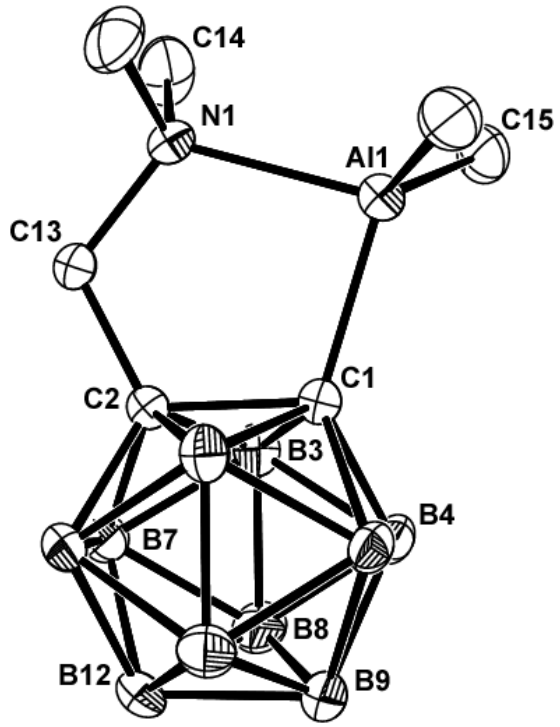

Figure S2. Molecular structure of **4**.