## Assembly of a Planar, Tricyclic B<sub>4</sub>N<sub>8</sub> Framework With *s*-Indacene Structure

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- Supplementary Information -

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 $^{1}$ H and  $^{11}$ B NMR Spectra of 1,2-dimethyl-3,5-diphenyl-4-methylamino-1,2,4-triaza-3,5-diborolidine (2) in C<sub>6</sub>D<sub>6</sub>



<sup>13</sup>C NMR Spectrum of 1,2-dimethyl-3,5-diphenyl-4-methylamino-1,2,4-triaza-3,5-diborolidine (**2**) in C<sub>6</sub>D<sub>6</sub>



<sup>1</sup>H and <sup>11</sup>B NMR Spectra of the dilithium salt (3) in THF-d<sub>8</sub>



Supplementary Material (ESI) for Chemical Communications This journal is (c) The Royal Society of Chemistry 2007  $^{13}$ C and  $^{7}$ Li NMR Spectra of the dilithium salt (3) in THF-d<sub>8</sub>



<sup>1</sup>H and <sup>11</sup>B NMR Spectra of the tricyclic tetrahydrazidotetraborane (4) in THF-d<sub>8</sub>



 $^{13}$ C NMR Spectrum of the tricyclic tetrahydrazidotetraborane (4) in THF-d<sub>8</sub>





**Fig. S1** Cyclovoltammogram of **4** in the presence of the internal standard  $[Cp_2Co]PF_6 ([Cp_2Co]^{0/+1}]$  with  $E^0 = -1.36$  V vs. ferrocene and -0.82 V vs. the SCE) at 200 ms scan rate. The measurements were performed in THF at an analyte concentration of 1 mM, and using 0.1 M [*n*Bu<sub>4</sub>N]PF<sub>6</sub> as a supporting electrolyte.



Potential (V vs. Ferrocene)

Fig. S2 Cyclovoltammogram of 4 in the absence of the internal standard at 50 ms scan rate. The measurements were performed in THF at an analyte concentration of 1 mM, and using 0.1 M  $[nBu_4N]PF_6$  as a supporting electrolyte.



Fig. S3 Occupied  $\pi$ -like Kohn-Sham orbitals of 4. For simplicity, orbitals are shown for a structure in which Me and Ph substituents attached to nitrogen and boron atoms have been replaced with hydrogen atoms.



**Fig. S4** Occupied  $\pi$ -symmetric Kohn-Sham  $\alpha$ -orbitals of open-shell singlet [4]<sup>2+</sup>. For simplicity, orbitals are shown for a structure in which Me and Ph substituents attached to nitrogen and boron atoms have been replaced with hydrogen atoms.



**Fig. S5** Occupied  $\pi$ -symmetric Kohn-Sham  $\beta$ -orbitals of open-shell singlet  $[4]^{2+}$ . For simplicity, orbitals are shown for a structure in which Me and Ph substituents attached to nitrogen and boron atoms have been replaced with hydrogen atoms.



**Fig. S6** Occupied  $\pi$ -symmetric Kohn-Sham  $\alpha$ -orbitals of triplet  $[4]^{2+}$ . For simplicity, orbitals are shown for a structure in which Me and Ph substituents attached to nitrogen and boron atoms have been replaced with hydrogen atoms.



**Fig. S7** Occupied  $\pi$ -symmetric Kohn-Sham  $\beta$ -orbitals of triplet  $[4]^{2+}$ . For simplicity, orbitals are shown for a structure in which Me and Ph substituents attached to nitrogen and boron atoms have been replaced with hydrogen atoms.

Optimized coordinates of  $\mathbf{4}$  and  $[\mathbf{4}]^{2+}$  in mol2 format:

0.0000

0.0000

## @<TRIPOS>MOLECULE

Singlet 4 58 62 1 SMALL NO\_CHARGES \*\*\*\* \*\*\*\* @<TRIPOS>ATOM 1 C 1.7111 1.9377 -1.1476 C.3 1 RES1 2 N 0.9526 1.1366 -0.2110 N.3 1 RES1

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9	С	-0.8248	3.7557	0.4627	C.3	1 RES1	0.0000
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11	В	-2.7152	0.7394	0.0786	В	1 RES1	0.0000
12	Ν	-2.5836	2.1629	0.0170	N.3	1 RES1	0.0000
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45 H	Η	7.1663	0.0649	-1.4792 H	1 RES1	0.0000
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47 H	Η	5.6863	2.4325	1.7690 H	1 RES1	0.0000
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55 H	Η	-7.1663	-0.0649	1.4792 H	1 RES1	0.0000
56 H	Η	-7.5238	-1.8285	-0.2220 H	1 RES1	0.0000
57 H	Η	-5.6863	-2.4325	-1.7690 H	1 RES1	0.0000
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J D 6 N	1 388/	0.0373	0.1201 D 0.1233 Npl	1 KLSI 2 1 DESI	0.0000
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7 N 8 C	-0.9031	-1.1403 2.1747	0.1452 N.5	1 DES1	0.0000
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11 C 12 N	1 388/	-0.1585	-0.1233 N n	13 1 RES1	0.0000
12 R 13 R	0.4753	-0.1303	-0.1255 N.p	1 RES1	0.0000
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38	Η	-3.5095	3.8266	-0.6261 H	1 RES1	0.0000
39	С	-4.4603	-0.8059	-1.0912 C.2	1 RES1	0.0000
40	С	-5.7150	-1.3849	-1.1998 C.2	1 RES1	0.0000
41	С	-6.6405	-1.2333	-0.1752 C.2	1 RES1	0.0000
42	С	-6.3155	-0.4904	0.9527 C.2	1 RES1	0.0000
43	С	-5.0690	0.1079	1.0530 C.2	1 RES1	0.0000
44	Η	-3.7540	-0.9236	-1.9081 H	1 RES1	0.0000
45	Η	-5.9749	-1.9517	-2.0864 H	1 RES1	0.0000
46	Η	-7.6197	-1.6908	-0.2579 H	1 RES1	0.0000
47	Η	-7.0372	-0.3739	1.7528 H	1 RES1	0.0000
48	Η	-4.8346	0.6841	1.9436 H	1 RES1	0.0000
49	С	4.4603	0.8059	1.0912 C.2	1 RES1	0.0000
50	С	5.7150	1.3849	1.1998 C.2	1 RES1	0.0000
51	С	6.6405	1.2333	0.1752 C.2	1 RES1	0.0000
52	С	6.3155	0.4904	-0.9527 C.2	1 RES1	0.0000
53	С	5.0690	-0.1079	-1.0530 C.2	1 RES1	0.0000
54	Η	3.7540	0.9236	1.9081 H	1 RES1	0.0000
55	Η	5.9749	1.9517	2.0864 H	1 RES1	0.0000
56	Η	7.6197	1.6908	0.2579 H	1 RES1	0.0000
57	Η	7.0372	0.3739	-1.7528 H	1 RES1	0.0000
58	Η	4.8346	-0.6841	-1.9436 H	1 RES1	0.0000
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6	2	5	1
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8	3	9	1
9	4	33	1
10	4	34	1
11	4	35	1
12	5	6	1
13	5	19	1
14	6	7	1
15	6	9	1

16	7	8	1	
17	7	13	1	
18	8	27	1	
19	8	28	1	
20	8	29	1	
21	9	10	1	
22	10	11	1	
23	10	12	1	
24	11	30	1	
25	11	31	1	
26	11	32	1	
27	12	13	1	
28	12	17	1	
29	13	14	1	
30	14	15	1	
31	14	18	1	
32	15	16	1	
33	15	17	1	
34	16	21	1	
35	16	22	1	
36	16	23	1	
37	17	20	1	
38	18	24	1	
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50	41	46	1	
51	42	43	1	
52	42	4/	1	
53	43	48	1	
54	49	50	1	
55 56	49	54	1	
56	50	51	1	
57 59	50	22 52	1	
58 50	51	52	1	
59	51	50 52	1	
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61 (2	52 52	5/	1	
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