

From *C,N*- and *N,N*-chelated chloroboranes to substituted 1*H*-2,1-benzazaboroles
and 1*H*-pyrrolo[1,2-*c*][1,3,2]diazaborolidines: A straightforward route
to five-membered rings containing B-N or N-B-N moiety

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SUPPLEMENTARY INFORMATION

full assignment of NMR data of compounds **1-18**

NMR spectroscopy

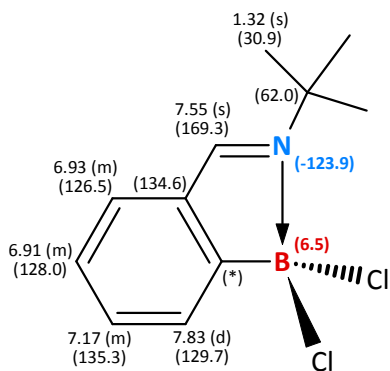
¹H, ¹¹B, ¹³C and ¹⁵N NMR spectra were recorded on a Bruker 500 Avance or a Bruker 400 MHz spectrometers, using a 5 mm tunable broad-band probe. Appropriate chemical shifts in ¹H and ¹³C NMR spectra were related to the residual signals of the solvent (C₆D₆: δ(¹H) = 7.16 ppm and δ(¹³C) = 128.39 ppm; CDCl₃: δ(¹H) = 7.27 ppm and δ(¹³C) = 77.23 ppm). ¹¹B NMR spectra were related to external standard B(OMe)₃ (δ(¹¹B) = 18.1 ppm) and ¹⁵N NMR spectra were related to external neat nitromethane (δ(¹⁵N) = 0.0 ppm). Deuterated solvents were dried by standard procedures. The full assignment of all signals in all measured NMR spectra was managed for all compounds with the help of various techniques including ¹H, ¹³C{¹H} APT, ¹H-¹H COSY, ¹H-¹³C HMQC and ¹H-¹³C HMBC experiments. ¹⁵N NMR chemical shifts were obtained from ¹H-¹⁵N HMBC spectra. Following NMR data includes multiplicities of signals in the ¹H NMR spectra. **Used abbreviations:** s = singlet, d = doublet, t = triplet, q = quartet, hep = heptet, dt = doublet of triplets, dq = doublet of quartets, td = triplet of doublets, tt = triplet of triplets, m = multiplet.

¹H, ¹¹B, (¹³C) and ¹⁵N NMR data (δ = [ppm]) in C₆D₆ (**1**, **2**, **4-18**) or in CDCl₃ (**3**) at 298 K

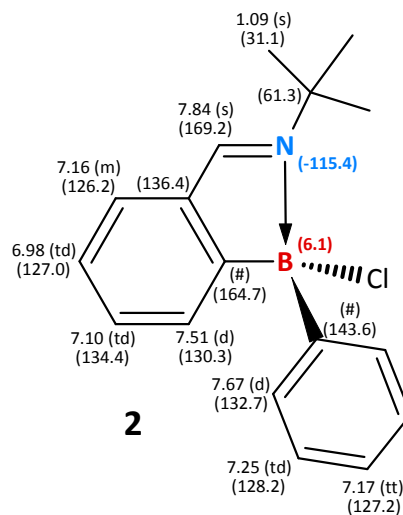
br. = broad signal

(*) Signal of this atom was not observed

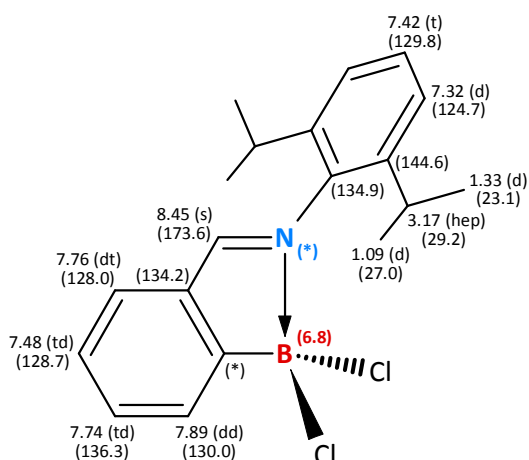
(#) Observation of signal of the carbon atom *7a* required application of 10⁵ pulses due to its
broadening



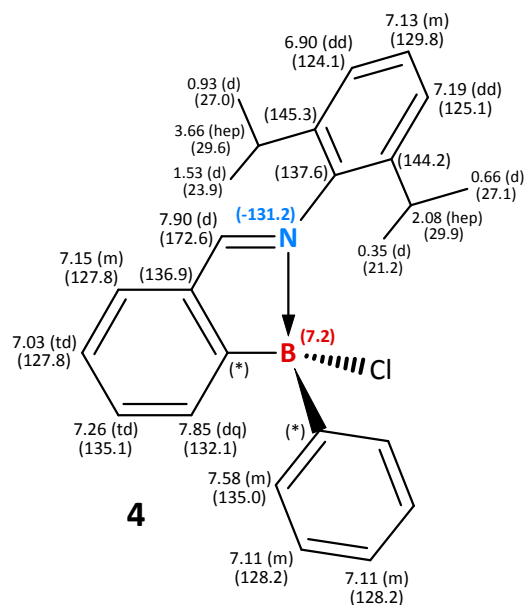
1



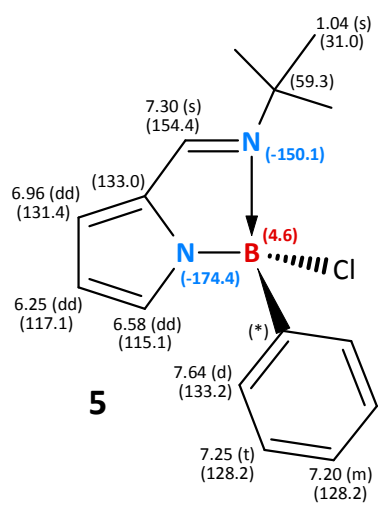
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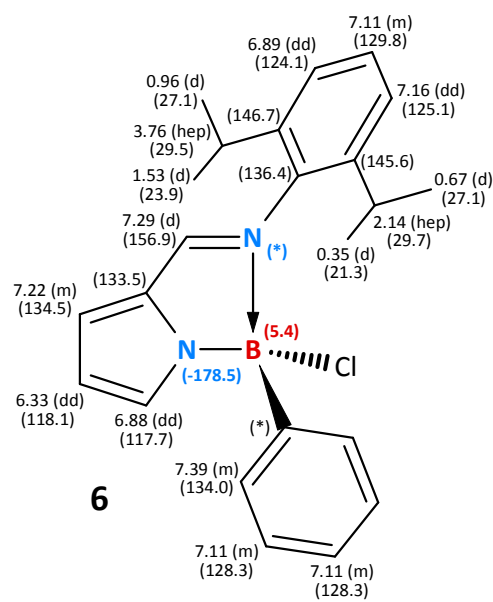
3



4



5



6

