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Supplementary Material

for the paper

An Inorganic Propellane with Central B−B Bond

Steffen Pospiech, Sarah Brough, Michael Bolte, Hans-Wolfram Lerner, Holger F. Bettinger and Matthias Wagner

Content:

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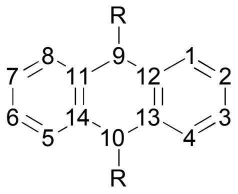
2. Single Crystal X-ray Structure Analyses of Compounds **1-5** and 1-Iso-propyl-2-mercaptoimidazole

1. Syntheses and NMR-spectroscopic Data of 9,10-Dilithio-9,10-dihydroanthracene, 1-*Iso*-propyl-2-mercaptoimidazole and Compounds 1-5

All reactions were carried out under an atmosphere of dry nitrogen using Schlenk techniques or in an argon-filled glovebox (MBraun). Pentane, hexane, benzene, toluene and THF were dried over Na/benzophenone; chloroform was dried over CaH_2. All reaction solvents were freshly distilled prior to use. C_6D_6 was dried over Na/K alloy; $CDCl_3$ was dried over CaH_2. NMR solvents were stored over molecular sieves (3 Å). NMR: Bruker AM-250, DPX-250, Avance300 and Avance400; all NMR spectra were measured at room temperature. Chemical shifts are referenced to residual solvent peaks (^1H / $^{13}C\{^1H\}$; C_6D_6: 7.16 ppm / 128.06 ppm; $CDCl_3$: 7.26 ppm / 77.16 ppm), external $BF_3 \cdot Et_2O$ ($^{11}B\{^1H\}$) or external $CFCl_3$ ($^{19}F\{^1H\}$). Abbreviations: s = singlet, d = doublet, dd = doublet of doublets, vtrd = virtual triplet of doublets, sep = septet, m = multiplet, br = broad, n.r. = not fully resolved, n.o. = signal not observed, mt = 2-mercaptoimidazolyl.

NMR resonances of the 9,10-dihydroanthracene framework have been assigned according to the following numbering scheme:



Synthesis of 9,10-Dilithio-9,10-dihydroanthracene. *n*-BuLi in hexane (2.20 M, 55.5 mL, 122.1 mmol) was added at r.t. to a solution of 9,10-dihydroanthracene (10.00 g, 55.48 mmol) in benzene (150 mL). The reaction mixture was heated to reflux temperature for 12 h, whereupon a dark purple precipitate formed. The mixture was allowed to cool to r.t., the precipitate was collected on a frit, washed with benzene (2 × 20 mL) and pentane (2 × 25 mL) and dried *in vacuo*. Yield: 8.75 g (82%).

Synthesis of 1. In a glovebox, neat $B_2(NMe_2)_2Cl_2$ (1.72 g, 9.52 mmol) was added slowly at r.t. via syringe to a suspension of 9,10-dilithio-9,10-dihydroanthracene (1.86 g, 9.68 mmol) in benzene (80 mL). The reaction mixture was stirred for 4 d. All insolubles were removed from the resulting suspension by filtration. The filtrate was evaporated under reduced pressure until a yellow oil remained from which **1** crystallised in the form of colourless blocks which were suitable for X-ray crystallography. Yield: 2.35 g (86%). ^1H NMR: δ_H(400.1 MHz; C_6D_6) 2.36 (6H, s, NMe_2), 2.64 (6H, s, NMe_2), 4.05 (2H, s, CH-9,10), 7.13 (4H, m, ArH-2,3,6,7), 7.28 (4H, m, ArH-1,4,5,8). ^{11}B NMR: δ_B(128.4 MHz; C_6D_6) 44.6 ($h_{1/2}$ = 400 Hz). ^{13}C NMR: δ_C(100.6 MHz; C_6D_6) 39.4 (NMe_2), 45.7

(NMe$_2$), 50.2 (br, C-9,10), 124.7 (C-1,4,5,8), 125.6 (C-2,3,6,7), 142.5 (C-11,12,13,14). Found: C, 74.77; H, 7.57; N, 9.58. $C_{18}H_{22}B_2N_2$ [288.00] requires C, 75.07; H, 7.70; N, 9.73.

Synthesis of 2. A solid mixture of **1** (58 mg, 0.20 mmol) and [H_2NMe_2]Br (25 mg, 0.20 mmol) was dissolved in chloroform (10 mL) and the solution was stirred for 3 h at r.t. The solvent was removed in vacuo to obtain a colourless solid residue of **2**. Yield: 75 mg (91%). Single crystals suitable for X-ray diffraction were obtained by gas-phase diffusion of hexane into a saturated solution of **2** in benzene. ^{1}H NMR: δ_H(300.0 MHz; CDCl$_3$) 1.51 (6H, d, $^3J_{HH}$ = 5.7 Hz, NH*Me*$_2$), 2.78 (6H, d, $^3J_{HH}$ = 5.7 Hz, NH*Me*$_2$), 3.02 (3H, s, NMe$_2$), 3.08 (3H, s, NMe$_2$), 3.86 (1H, s, CH-9 or 10), 4.16 (1H, s, CH-9 or 10), 7.06 (4H, m, ArH), 7.19 (2H, m, ArH), 7.24 (2H, m, ArH), 7.55 (2H, br, N*H*Me$_2$). ^{11}B NMR: δ_B(96.3 MHz; CDCl$_3$) 1.8 ($h_{1/2}$ = 300 Hz), 47.0 ($h_{1/2}$ = 800 Hz). ^{13}C NMR: δ_C(100.6 MHz; CDCl$_3$) 39.3 (NHMe$_2$), 40.4 (NMe$_2$), 42.9 (NHMe$_2$), 43.9 (C-9 or 10)*, 45.8 (NMe$_2$), 49.8 (C-9 or 10)*, 124.9, 125.0, 125.2, 125.7 (ArC-1 to 8), 142.0, 143.0 (ArC-11,12,13,14). *) *Note*: This resonance was broadened beyond detection in the 1D ^{13}C{^{1}H} NMR spectrum; we located the signal through its cross peak in the ^{1}H-^{13}C HMBC experiment. A correct elemental analysis of **2** was not obtained, because microcrystalline samples were always contaminated with small amounts of [H_2NMe_2]Br; the amount of single crystalline material was not sufficient to perform an elemental analysis.

Synthesis of 3. Ethereal HCl (0.91 M, 0.72 mL, 0.66 mmol) was added at −10 °C via syringe to a solution of **1** (95 mg, 0.33 mmol) in chloroform (15 mL). The reaction mixture was stirred at −10 °C for 80 min and then allowed to warm to r.t. From the resulting colourless solution, the solvent was removed in vacuo to obtain a colourless solid residue of **3**. Single crystals suitable for X-ray diffraction were grown by gas-phase diffusion of hexane into a saturated solution of **3** in chloroform. Yield: 103 mg (87%).

^{1}H NMR: δ_H(250.1 MHz; CDCl$_3$) 2.68 (6H, d, $^3J_{HH}$ = 5.8 Hz, NH*Me*$_2$), 2.77 (6H, d, $^3J_{HH}$ = 5.8 Hz, NH*Me*$_2$), 3.27 (2H, br, N*H*Me$_2$), 3.56 (2H, s, CH-9,10), 6.98 (2H, vtrd, $^3J_{HH}$ = 7.2 Hz, $^4J_{HH}$ = 1.4 Hz, ArH-2,6 or 3,7), 7.04 (2H, vtrd, $^3J_{HH}$ = 7.2 Hz, $^4J_{HH}$ = 1.4 Hz, ArH-2,6 or 3,7), 7.10 (2H, dd, $^3J_{HH}$ = 7.2 Hz, $^4J_{HH}$ = 1.4 Hz, ArH-1,5 or 4,8), 7.22 (2H, dd, $^3J_{HH}$ = 7.2 Hz, $^4J_{HH}$ = 1.4 Hz, ArH-1,5 or 4,8). ^{11}B NMR: δ_B(80.3 MHz; CDCl$_3$) 5.2 ($h_{1/2}$ = 400 Hz). ^{13}C NMR: δ_C(75.4 MHz; CDCl$_3$) 37.1 (NHMe$_2$), 41.5 (NHMe$_2$), 51.2 (br, C-9,10), 123.3 (ArC-1,5 or 4,8), 124.2 (ArC-2,6 or 3,7), 124.6 (ArC-2,6 or 3,7), 126.1 (ArC-1,5 or 4,8), 141.5, 145.7 (ArC-11,12,13,14). Found: C, 59.70; H, 6.84; N, 7.82. $C_{18}H_{24}B_2Cl_2N_2$ [360.91] requires C, 59.90; H, 6.70; N, 7.76.

Synthesis of 4. Neat F_3CCOOH (37 μL, 55 mg, 0.48 mmol) was added at r.t. via Hamilton syringe to a stirred solution of **1** (69 mg, 0.24 mmol) in benzene (12 mL). After 30 min, the mixture was freeze-dried and a colourless solid residue remained in the flask. Yield: 114 mg (92%). Crystals suitable for X-ray analysis were grown by gas-phase diffusion of hexane into a saturated solution of **4** in benzene.

^{1}H NMR: δ_H(400.1 MHz; C_6D_6) 1.54 (6H, d, $^3J_{HH}$ = 5.8 Hz, NH*Me*$_2$), 1.93 (6H, d, $^3J_{HH}$ = 5.8 Hz, NH*Me*$_2$), 3.66 (2H, s, CH-9,10), 4.45 (2H, br, N*H*Me$_2$), 6.98 (2H, m, ArH), 7.09 (4H, m, ArH), 7.29 (2H, m, ArH). ^{11}B NMR: δ_B(128.4 MHz; C_6D_6) 6.8 ($h_{1/2}$ = 300 Hz). ^{13}C NMR: δ_C(100.6 MHz; C_6D_6) 36.4 (NHMe$_2$), 39.1 (NHMe$_2$), 48.1 (C-9,10), 123.5 (ArC), 125.0 (3 overlapping signals; ArC), 141.5, 143.9 (ArC-11,12,13,14), n.o. (CF_3, COO). ^{19}F NMR: δ_F(282.3 MHz; C_6D_6) −75.9. *Note*: Due to the poor solubility of **5**, the 1D ^{13}C{^{1}H} NMR spectrum suffered from a low signal-to-noise ratio; we therefore located the ^{13}C signals through their cross peaks in the ^{1}H-^{13}C HMBC experiment. Found: C, 47.80; H, 3.98; N, 5.15. $C_{22}H_{24}B_2F_6N_2O_4$ [516.05] · 0.4 $CHCl_3$ [119.38] requires C, 47.72; H, 4.36; N, 4.97. *Note*: Upon prolonged storage under vacuum, the compound tends to loose some of its chloroform solvate (NMR spectroscopic control).

Synthesis of 1-*Iso*-propyl-2-mercaptoimidazole (Hmt^{iPr}). The compound is literature known,[1S-3S] however, a full NMR characterisation as well as an X-ray crystal structure analysis was still missing and is therefore provided below.

Neat isopropyl isothiocyanate (2.5 mL, 2.37 g, 23.4 mmol) was added slowly via syringe at 0 °C to a solution of aminoacetaldehyde diethyl acetal (3.4 mL, 3.11 g, 23.4 mmol) in THF (50 mL). The reaction mixture was heated to reflux temperature for 4 h and afterwards allowed to cool to r.t. From the resulting colourless solution, the solvent was removed in vacuo to obtain an oily residue. Sulfuric acid (10%, 90 mL) was added and the resulting mixture was heated to reflux temperature for 21 h, whereupon a red solution formed. After neutralisation with aqueous NaOH, the crude product of Hmt^{iPr} was extracted into dichloromethane (3 × 100 mL) and the combined organic phases were dried over $MgSO_4$. After filtration, the solvent was removed from the filtrate under reduced pressure to yield a light orange solid residue. Recrystallisation from hot toluene gave light orange crystals of Hmt^{iPr} suitable for X-ray diffraction. Yield: 1.8 g (54%).

^{1}H NMR: δ_H(250.1 MHz; $CDCl_3$) 1.37 (6H, d, $^3J_{HH}$ = 6.7 Hz, CH*Me*$_2$), 5.04 (2H, sep, $^3J_{HH}$ = 6.7 Hz, C*H*Me$_2$), 6.75 (2H, m, CH-mt), 11.66 (1H, br, NH). ^{13}C NMR: δ_C(62.9 MHz; $CDCl_3$) 22.1 (CH*Me*$_2$), 48.2 (*C*HMe$_2$), 114.0, 114.7 (CH-mt), n.o. (CS).

[1S] R. G. Jones, E. C. Kornfeld, K. C. McLaughlin and R. C. Anderson, *J. Am. Chem. Soc.* 1949, **71**, 4000-4002.
[2S] G. Assef, J. Kister, J. Metzger, R. Faure and E. J. Vincent, *Tetrahedron Lett.* 1976, **17**, 3313-3316.
[3S] J. Kister, G. Assef, G. Mille and J. Metzger, *Can. J. Chem.* 1979, **57**, 813-821.

Synthesis of 5. A solid mixture of **1** (216 mg, 0.75 mmol) and Hmt^{iPr} (213 mg, 1.50 mmol) was dissolved in benzene (30 mL), the solution was sealed in an ampoule and kept at 85 °C for 7 d. Afterwards, the sample was freeze-dried to obtain a light yellow solid residue, which was recrystallised from hot toluene to obtain colourless blocks of **5**. Yield: 202 mg (56%).

^{1}H NMR: δ_H(400.1 MHz; C_6D_6) 0.52 (6H, d, $^3J_{HH}$ = 6.7 Hz, CH*Me*$_2$), 0.54 (6H, d, $^3J_{HH}$ = 6.7 Hz, CH*Me*$_2$), 3.70 (2H, sep, $^3J_{HH}$ = 6.7 Hz, C*H*Me$_2$), 4.40 (2H, s, CH-9,10), 5.82 (2H, d, $^3J_{HH}$ = 2.0 Hz, CH-mt), 6.54 (2H, d, $^3J_{HH}$ = 2.0 Hz, CH-mt), 6.96 (2H, vtrd, $^3J_{HH}$ = 7.3 Hz, $^4J_{HH}$ = 1.2 Hz, ArH-2,6 or

3,7), 7.08 (2H, dd, $^3J_{HH}$ = 7.3 Hz, $^4J_{HH}$ = n.r., ArH-1,5 or 4,8), 7.13 (2H, vtrd, $^3J_{HH}$ = 7.3 Hz, $^4J_{HH}$ = 1.2 Hz, ArH-2,6 or 3,7), 7.60 (2H, dd, $^3J_{HH}$ = 7.3 Hz, $^4J_{HH}$ = n.r., ArH-1,5 or 4,8). ^{11}B NMR: δ_B(128.4 MHz; C_6D_6) 6.2 ($h_{1/2}$ = 350 Hz). ^{13}C NMR: δ_C(100.6 MHz; C_6D_6) 20.9 (CH*Me*$_2$), 21.7 (CH*Me*$_2$), 48.2 (br, C-9,10), 50.0 (*C*HMe$_2$), 116.7, 120.8 (CH-mt), 123.3, 123.4 (ArC-2,3,6,7), 123.8, 125.6 (ArC-1,4,5,8), 144.5, 145.8 (ArC-11,12,13,14), 160.4 (CS). Found: C, 64.67; H, 5.84; N, 11.37; S, 13.31. $C_{26}H_{28}B_2N_4S_2$ [482.26] requires C, 64.75; H, 5.85; N, 11.62; S, 13.30.

2. Single Crystal X-ray Structure Analyses of Compounds 1-5 and 1-Iso-propyl-2-mercaptoimidazole

Crystal Structure Analyses. Data were collected on a STOE IPDS II two-circle diffractometer with graphite-monochromated MoK_α radiation. Empirical absorption corrections were performed for all structures but **1** using the MULABS[4S] option in PLATON[5S]. The structures were solved by direct methods using the program SHELXS[6S] and refined against F^2 with full-matrix least-squares techniques using the program SHELXL-97[7S]. The H atoms bonded to N in **2**, **3**, **4** and Hmt^{iPr} were freely refined. In **4**, one CF_3 group is disordered over three positions with site occupation factors of 0.293(3), 0.407(7) and 0.300(7).

4S R. H. Blessing, *Acta Cryst.* 1995, **A51**, 33-38.
5S A. L. Spek, *J. Appl. Cryst.* 2003, **36**, 7-13.
6S G. M. Sheldrick, *Acta Cryst.* 1990, **A46**, 467-473.
7S G. M. Sheldrick, *SHELXL-97. A Program for the Refinement of Crystal Structures*, Universität Göttingen, Göttingen, Germany, 1997.

Crystal data of **1**: $C_{18}H_{22}B_2N_2$, M = 288.00 g mol^{-1}, orthorhombic, a = 12.4867(7) Å, b = 8.0814(6) Å, c = 16.3838(9) Å, V = 1653.29(18) Å^3, T = 173(2) K, space group *Pbcn*, Z = 4, μ(Mo-K$_\alpha$) = 0.066 mm^{-1}, 26385 reflections measured, 1548 unique (R_{int} = 0.0660) which were used in all calculations. Final R values: $R1$ = 0.0443, $wR(F^2)$ = 0.0920 ($I > 2\sigma(I)$); $R1$ = 0.0752, $wR(F^2)$ = 0.1024 (all data).

Crystal data of **2**: $C_{20}H_{30}B_2BrN_3$, M = 414.00 g mol^{-1}, monoclinic, a = 18.1734(15) Å, b = 9.3798(7) Å, c = 24.6564(18) Å, β = 95.039(6)°, V = 4186.8(6) Å^3, T = 173(2) K, space group *C*2/*c*, Z = 8, μ(Mo-K$_\alpha$) = 1.972 mm^{-1}, 13015 reflections measured, 3932 unique (R_{int} = 0.0627) which were used in all calculations. Final R values: $R1$ = 0.0370, $wR(F^2)$ = 0.0810 ($I > 2\sigma(I)$); $R1$ = 0.0569, $wR(F^2)$ = 0.0867 (all data).

Crystal data of **3**: $C_{18}H_{24}B_2Cl_2N_2$, M = 360.91 g mol^{-1}, orthorhombic, a = 15.8266(9) Å, b = 12.0793(8) Å, c = 9.9030(6) Å, V = 1893.2(2) Å^3, T = 173(2) K, space group $Pna2_1$, Z = 4, μ(Mo-K$_\alpha$) = 0.344 mm^{-1}, 7304 reflections measured, 3272 unique (R_{int} = 0.0368) which were used in all calculations. Final R values: $R1$ = 0.0262, $wR(F^2)$ = 0.0569 ($I > 2\sigma(I)$); $R1$ = 0.0305, $wR(F^2)$ = 0.0578 (all data). Flack-x-parameter = 0.05(4).

Crystal data of **4**: $C_{22}H_{24}B_2F_6N_2O_4 \cdot 0.5\ CHCl_3$, M = 575.74 g mol^{-1}, triclinic, a = 12.1883(6) Å, b = 15.1818(8) Å, c = 16.1826(8) Å, α = 110.842(4)°, β = 106.505(4)°, γ = 98.129(4)°, V = 2583.1(2) Å^3, T = 173(2) K, space group P-1, Z = 4, μ(Mo-K$_\alpha$) = 0.276 mm^{-1}, 30575 reflections measured, 9116 unique (R_{int} = 0.0708) which were used in all calculations. Final R values: $R1$ = 0.0569, $wR(F^2)$ = 0.1500 ($I > 2\sigma(I)$); $R1$ = 0.0748, $wR(F^2)$ = 0.1597 (all data).

Crystal data of **5**: $C_{26}H_{28}B_2N_4S_2$, M = 482.26 g mol^{-1}, orthorhombic, a = 26.6672(6) Å, b = 8.5931(2) Å, c = 10.7151(2) Å, V = 2455.41(9) Å^3, T = 173(2) K, space group $Pca2_1$, Z = 4, μ(Mo-K$_\alpha$) = 0.240 mm^{-1}, 29599 reflections measured, 5641 unique (R_{int} = 0.0480) which were used in all calculations. Final R values: $R1$ = 0.0410, $wR(F^2)$ = 0.1090 ($I > 2\sigma(I)$); $R1$ = 0.0424, $wR(F^2)$ = 0.1099 (all data). Flack-x-parameter = −0.05(6).

Crystal data of **Hmt$^{i\mathrm{Pr}}$**: $C_6H_{10}N_2S$, M = 142.22 g mol^{-1}, monoclinic, a = 10.5400(8) Å, b = 10.0952(6) Å, c = 14.5231(13) Å, β = 94.236(7)°, V = 1541.1(2) Å^3, T = 173(2) K, space group $P2_1/c$, Z = 8, μ(Mo-K$_\alpha$) = 0.336 mm^{-1}, 10324 reflections measured, 2880 unique (R_{int} = 0.0473) which were used in all calculations. Final R values: $R1$ = 0.0342, $wR(F^2)$ = 0.0881 ($I > 2\sigma(I)$); $R1$ = 0.0437, $wR(F^2)$ = 0.0919 (all data).

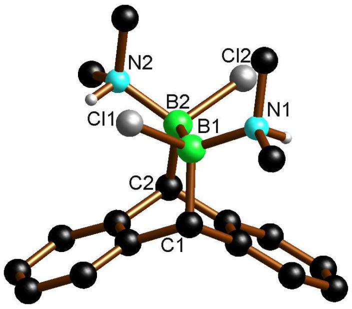


Figure S1. Molecular structure and numbering scheme of compound **3**; protons attached to carbon atoms are omitted for clarity. Selected bond lengths [Å], atom···atom distances [Å], bond angles [°], and torsion angle [°]: B(1)−B(2) = 1.757(3), B(1)−N(1) = 1.627(3), B(1)−C(1) = 1.653(3), B(1)−Cl(1) = 1.931(2), B(2)−N(2) = 1.626(3), B(2)−C(2) = 1.655(3), B(2)−Cl(2) = 1.929(2), av. H···Cl (intramolecular) = 2.87; N(1)−B(1)−Cl(1) = 105.0(1), C(1)−B(1)−B(2) = 105.9(1), N(1)−B(1)−B(2) = 116.1(2), N(2)−B(2)−Cl(2) = 104.4(1), C(2)−B(2)−B(1) = 106.4(2), N(2)−B(2)−B(1) = 113.3(1), av. N−H···Cl (intramolecular) = 109.9; N(1)−B(1)−B(2)−N(2) = −118.9(2).

Compound **4** crystallises with two crystallographically independent molecules, **4** and $\mathbf{4}_\mathbf{A}$, in the asymmetric unit. A remarkable difference between **4** and $\mathbf{4}_\mathbf{A}$ lies in the fact that $\mathbf{4}_\mathbf{A}$ features only one intramolecular NH−O hydrogen bond, whereas **4** contains two.

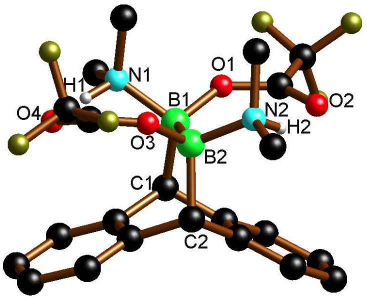


Figure S2$_\mathbf{A}$. Molecular structure and numbering scheme of compound **4**; protons attached to carbon atoms are omitted for clarity, only one of the three positions of the disordered CF_3 group is shown. Selected bond lengths [Å], bond angles [°] and torsion angle [°]: B(1)−B(2) = 1.799(3), B(1)−N(1) = 1.615(3), B(1)−C(1) = 1.664(3), B(1)−O(1) = 1.551(3), B(2)−N(2) = 1.609(3), B(2)−C(2) = 1.661(3), B(2)−O(3) = 1.547(3), av. H−O = 2.07; N(1)−B(1)−B(2) = 115.5(2), C(1)−B(1)−B(2) = 105.2(2), O(1)−B(1)−B(2) = 122.4(2), N(1)−B(1)−O(1) = 98.5(2), N(2)−B(2)−B(1) = 115.5(2), C(2)−B(2)−B(1) = 105.3(2), O(3)−B(2)−B(1) = 120.6(2), N(2)−B(2)−O(3) = 99.1(2); N(1)−B(1)−B(2)−N(2) = −116.3(2).

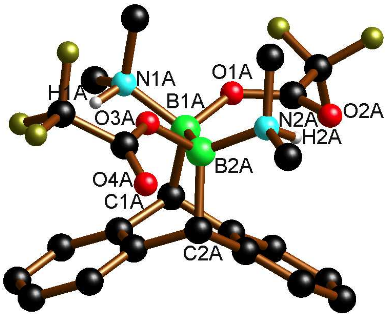


Figure S2$_\mathbf{B}$. Molecular structure and numbering scheme of compound $\mathbf{4}_\mathbf{A}$; protons attached to carbon atoms are omitted for clarity. Selected bond lengths [Å], bond angles [°] and torsion angle [°]: B(1A)−B(2A) = 1.781(3), B(1A)−N(1A) = 1.633(3), B(1A)−C(1A) = 1.655(3), B(1A)−O(1A) = 1.545(3), B(2A)−N(2A) = 1.614(3), B(2A)−C(2A) = 1.659(3), B(2A)−O(3A) = 1.545(3), H(2A)−O(2A) = 2.02(3); N(1A)−B(1A)−B(2A) = 111.3(2), C(1A)−B(1A)−B(2A) = 106.0(2), O(1A)−B(1A)−B(2A) = 124.7(2), N(1A)−B(1A)−O(1A) = 99.8(2), N(2A)−B(2A)−B(1A) = 116.2(2), C(2A)−B(2A)−B(1A) = 105.6(2), O(3A)−B(2A)−B(1A) = 107.2(2), N(2A)−B(2A)−O(3A) = 106.7(2); N(1A)−B(1A)−B(2A)−N(2A) = −115.8(2).

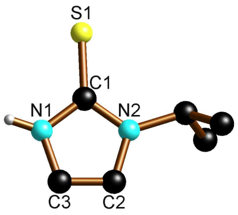


Figure S3. Molecular structure and numbering scheme of compound **Hmt^{iPr}**; protons attached to carbon atoms are omitted for clarity. Selected bond lengths [Å] and bond angles [°]: C(1)−S(1) = 1.698(2), C(1)−N(1) = 1.352(2), C(1)−N(2) = 1.348(2), C(2)−N(2) = 1.391(2), C(2)−C(3) = 1.335(3), C(3)−N(1) = 1.378(2); N(1)−C(1)−N(2) = 105.8(1), N(1)−C(1)−S(1) = 126.7(1), N(2)−C(1)−S(1) = 127.5(1), C(1)−N(1)−C(3) = 110.4(1), C(1)−N(2)−C(2) = 109.5(1).