Electronic supplementary information

Decaborane anion tautomerism: ion pairing and proton transfer control

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**Figure S1** Packing of salt 1 along the $bc$ plane. H(7)···H(7). The cations and anions form chains along the $a$ axis; contacts between inversion-centre related chains are highlighted in orange.
Figure S2 500 MHz $^1$H-$^{11}$B NMR spectra of salt 1 in CD$_2$Cl$_2$ at 178 K.

Figure S3 Variable temperature (VT): 500 MHz $^1$H-$^{11}$B NMR spectra of salt 1 in CDCl$_3$. The signals of neutral B$_{10}$H$_{14}$ and anionic [B$_{10}$H$_{13}$]$^-$ are highlighted in blue squares and red triangles, respectively.
Figure S4 Variable temperature (VT): 160 MHz $^{11}$B-$^1$H NMR spectra of salt 1 in CDCl$_3$. The signals of neutral B$_{10}$H$_{14}$ and anionic [B$_{10}$H$_{13}$]$^-$ are highlighted in blue squares and red triangles, respectively.

**Thermodynamic data**

**Table S1** The equilibrium ratios of the anionic versus the neutral species measured by $^1$H-$^{11}$B NMR

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<th>Temperature (K)</th>
<th>1/T(K) $10^3$</th>
<th>$K_{eq} = [B_{10}H_{13}^-]/[B_{10}H_{14}][PS]$</th>
<th>ln $K_{eq}$</th>
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$\Delta G = -RT \ln K_{eq}$ (R = 8.314 J K$^{-1}$ mol$^{-1}$)

$\Delta G = \Delta H - T\Delta S$

ln $K_{eq} = - \Delta H/RT + \Delta S/R$

$- \Delta H/R = 6975.2$; $\Delta H = -57.992$ kJ K$^{-1}$ mol$^{-1}$ = $-13.85 \pm 0.25$ kcal K$^{-1}$ mol$^{-1}$

$\Delta S/R = -18.293$; $\Delta S = -152.089$ J K$^{-1}$ mol$^{-1}$ = $-36.33 \pm 0.25$ calK$^{-1}$ mol$^{-1}$

$\Delta G_{298} = -13,850 - 298 \times (-36.33) = -3.02 \pm 0.25$ kcal mol$^{-1}$
Calculation of free energy of activation by the coalescence temperature:

*at The B-H terminal resonances:*

δ_H at +2.91 (2H), +2.86 (1H), +2.53 (1H) and +2.43 (1H ). These peaks coalesce in pairs at 303 K in a 11.7467 Tesla magnetic field. The fraction of these nuclei at 243 K is: \( P_A = 0.50 \) and \( P_B = 0.50 \), \( \Delta P = 0.00 \) equal populated sites, and \( \delta \nu = 238.5 \) Hz for the peaks of relative intensity two, and 162.3 Hz for the peaks of intensity one.

\[
\Delta G^\ddagger = -RT_c[\ln(\pi\delta \nu h/2^{1/2}\kappa_B T_c)] = RT_c[22.8 + \ln(T_c/\delta \nu)] = 8.3145 \times 303[22.8 + \ln(303/238)] = 58.1 \text{ kJ mol}^{-1} = 13.9 \text{ kcal mol}^{-1}.
\]

\[ R = 8.3145 \text{ J K}^{-1} \text{ mol}^{-1}, \]
\[ h = 6.626 \times 10^{-34} \text{ J s}, \]
\[ \kappa_B = 1.381 \times 10^{-23} \text{ J/K} \]

*at the B–H–B proton nuclei:*


\( P_A, P_B = \) factional populations of nuclei in sites A and B: at 243 K \( P_A = 1/3 \) and \( P_B = 2/3 \); \( \Delta P = 0.33 \). These correspond to the signals of relative intensity ratio at –2.70 and –3.54 ppm.

\[
\delta \nu = 422 \text{ Hz, } T_c = 318 \text{ K and } X = 2.0823
\]

\[
\Delta G_A^\ddagger = 4.57T_c[10.62 + \log X/2(1 + \Delta P) + \log T_c/\delta \nu]
\]

\[
\Delta G_B^\ddagger = 4.57T_c[10.62 + \log X/2(1 + \Delta P) + \log T_c/\delta \nu]
\]

\[
\Delta G_A^\ddagger = 4.57 \times 318[10.62 + \log 2.0823/2(1 + 0.33) + \log 318/422] = 4.57 \times 318[10.62 - 0.43] = 14.8 \text{ kcal mol}^{-1}.
\]

\[
\Delta G_A^\ddagger = 4.57 \times 318[10.62 + \log 2.0823/2(1 + 0.33) + \log 318/422] = 4.57 \times 318[10.62 - 0.73] = 14.4 \text{ kcal mol}^{-1}.
\]
Boron-11 selective decoupling experiments

Figure S5 Subtraction of the off-decoupled spectrum, $^1$H-{$^{11}$B(off)}, from the Broad Band (BB) decoupled spectrum, $^1$H-{$^{11}$B(BB)} (bottom trace); and subtractions of the $^1$H-{$^{11}$B(off)} spectrum from the $^{11}$B-selectively decoupled spectra, $^1$H-{$^{11}$B($\delta_B$)} for compound 1.

Figure S6 Subtraction of the off-decoupled spectrum, $^1$H-{$^{11}$B(off)}, from the Broad Band (BB) decoupled spectrum, $^1$H-{$^{11}$B(BB)} (bottom trace); and subtractions of the
$^1$H-$^{11}$B(off)) spectrum from the $^{11}$B-selectively decoupled spectra, $^1$H-$^{11}$B($\delta_B$)) for decaborane, nido-$^{10}$B$_{10}$H$_{14}$.

**Figure S7** Subtraction of the off-decoupled spectrum, $^1$H-$^{11}$B(off)), from the Broad Band (BB) decoupled spectrum, $^1$H-$^{11}$B(BB)) (bottom trace); and subtractions of the $^1$H-$^{11}$B(off)) spectrum from the $^{11}$B-selectively decoupled spectra, $^1$H-$^{11}$B($\delta_B$)) for the pyridine adduct, 6,9-(py)$_2$-arachno-$^{10}$B$_{10}$H$_{12}$.

**Diffusion coefficients:**

The following equation describes the situation for random isotropic diffusion. $I$ is the intensity of a peak, $D$ is the diffusivity, $G$ is the pulse gradient strength, $\delta$ is the length of the gradient pulse, and $\Delta$ is the diffusion time.

$$I = I_0 \exp\left[-D\gamma^2 G^2 \delta^2 (\Delta/3)\right]$$

Plotting $I$ vs. $G$ for a given peak gives a diffusion curve which is fit by TopSpin software to give $D$. 
Figure S8. *TopSpin* display after fitting with *SimFit* (*T1/T2* Analysis). The fitting curve for the peak at +3.24 ppm of salt 1 in CD2Cl2 is shown. The plot is ideal, and the fit is, therefore, reliable. This peak corresponds to the [PSH]+ cation.

Figure S9. *TopSpin* display after fitting with *SimFit* (*T1/T2* Analysis). The fitting curve for the peak at +0.34 ppm of salt 1 in CD2Cl2 is shown. The plot is not ideal, and the fit is not as reliable as the others. This peak corresponds to the [B10H13]− anion.
Figure S10. TopSpin display after fitting with SimFit ($T_1/T_2$ Analysis). The fitting curve for the peak at +6.98 ppm of pure PS in CD$_2$Cl$_2$ is shown. The plot is ideal, and the fit is, therefore, reliable.

Figure S11. TopSpin display after fitting with SimFit ($T_1/T_2$ Analysis). The fitting curve for the peak at -2.03 ppm of pure decaborane, B$_{10}$H$_{14}$, in CD$_2$Cl$_2$ is shown.
Figure S12. TopSpin display after fitting with SimFit ($T_1/T_2$ Analysis). The fitting curve for the peak at +0.23 ppm of salt 1 in CD$_3$CN is shown. The peak corresponds to the polyhedral anion. The plot is not ideal, and the fit is not as reliable as others in this study.

Figure S13. TopSpin display after fitting with SimFit ($T_1/T_2$ Analysis). The fitting curve for the peak at +7.91 ppm of salt 1 in CD$_3$CN is shown. The peak corresponds to PSH$^+$. The plot is ideal, and the fit is reliable.
Figure S14. TopSpin display after fitting with SimFit ($T_1/T_2$ Analysis). The fitting curve for the peak at +7.00 ppm of PS in CD$_3$CN is shown. The plot is ideal, and the fit is reliable.
Figure S15. TopSpin display after fitting with SimFit ($T_1/T_2$ Analysis). The fitting curve for the peak at +0.75ppm of salt 1 in CD$_3$CN is shown. This peak corresponds to the polyhedral anion. Plot too short, the fit is not good enough so the value of the diffusion coefficient is not as reliable as the measured for PS in CD$_3$CN.

Calculation of hydrodynamic radius.

Stokes-Einstein relation:

$$r_H = kT / 6\eta\pi D$$

$$k = 1.38064852(79) \times 10^{-23} \text{ JK}^{-1}$$

$T$ = temperature (K)

$\eta$ = viscosity of the solvent

Viscosity of dichlomethane = 0.413 cP (25 °C)

Viscosity of dichlomethane = 0.413 cP (25 °C)
Natural Atomic Charges (NBO)

Figure S16. Calculated Natural Atomic Charges in the \([\text{B}_{10}\text{H}_{13}]^-\) anion of salt 1 and in decaborane. For clarity, it is only shown the proton of the organic cation.
Tables of the optimized geometries (Cartesian coordinates, in Angstroms). Sum of electronic and thermal Free Energies (in Hartrees) in parenthesis.

Table S2. \([PSH][B_{10}H_{13}]\) (-910.588615): zero energy reference \(1C_{1-a}\) in Figure 8, main text.

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### Table S3. [PSH][B\textsubscript{10}H\textsubscript{13}] (-910.588534): zero reference energy 1C\textsubscript{1}b in Figure 8, main text.

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Table S4. [PSH][B_{10}H_{13}] (-910.582221): ion pair, 1C_{1-c}, TS +4.0 kcal mol\(^{-1}\) above the lowest energy pairs in Figure 8, main text.

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Table S5. [PSH][B$_{10}$H$_{13}$] (-910.58004800): ion pair, 1C$_{ex-a}$, +5.4 kcal mol$^{-1}$ above the lowest energy pair in Figure 8, main text.

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Table S5. [PSH][B$_{10}$H$_{13}$] (-910.58004800): ion pair, 1C$_{ex-a}$, +5.4 kcal mol$^{-1}$ above the lowest energy pair in Figure 8, main text.
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### Table S6. [PSH][B_{10}H_{13}] (-910.57801): ion pair, 1C_{a-b}, +6.6 kcal mol\(^{-1}\) above the lowest energy pair in Figure 8, main text.

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Cartesian coordinates (in Angstroms) corresponding to the Transition States calculated for the H-tautomerisms of nido-[B₁₀H₁₃]. Energies (in Hartrees) in parenthesis.

Table S8. [PSH][B₁₀H₁₃] (-910.577951): TS +6.7 kcal mol⁻¹ above the lowest energy pair in Figure 5, main text.

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Table S9. [PSH][B_{10}H_{13}] \((-910.566276): \text{TS} +14.0 \text{ kcal mol}^{-1}\) above the lowest energy pair in Figure 6, main text.
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