Supporting Information

Synthesis and Fluoride Binding Properties of Tris-pyridinium Borane

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Table S1. Crystallographic data and parameters for **2a**.

Compound	**2a**
formula	C39H36BN3
formula weight	557.52
crystal system	Monoclinic
space group	$P2_1/n$
a (Å)	12.3378(11)
b (Å)	15.0201(13)
c (Å)	18.1761(16)
α (°)	90.00
β (°)	109.641(4)
γ (°)	90.00
V (Å^3)	3172.3(5)
Z	4
ρ_{calc} (g cm^{-3})	1.167
μ (mm^{-1})	0.068
F(000)	1184
T (K)	296(2)
scan mode	ϕ and ω
hkl range	$-12 \rightarrow +12$, $-15 \rightarrow +13$, $-18 \rightarrow +18$
measd reflns	24378
unique reflns [R_{int}]	4652 [0.0773]
reflns used for refinement	4652
refined parameters	394
R1[a] (I > 2σ(I))	0.0465
wR2[b] all data	0.1154
GOF on F^2	1.004
ρ_{fin} (max/min) (e Å^{-3})	0.123, –0.112

[a] $R1 = \sum||Fo| - |Fc||/\sum|Fo|$. [b] $wR2 = \{[\sum w(Fo^2 - Fc^2)^2]/[\sum w(Fo^2)^2]\}^{1/2}$.

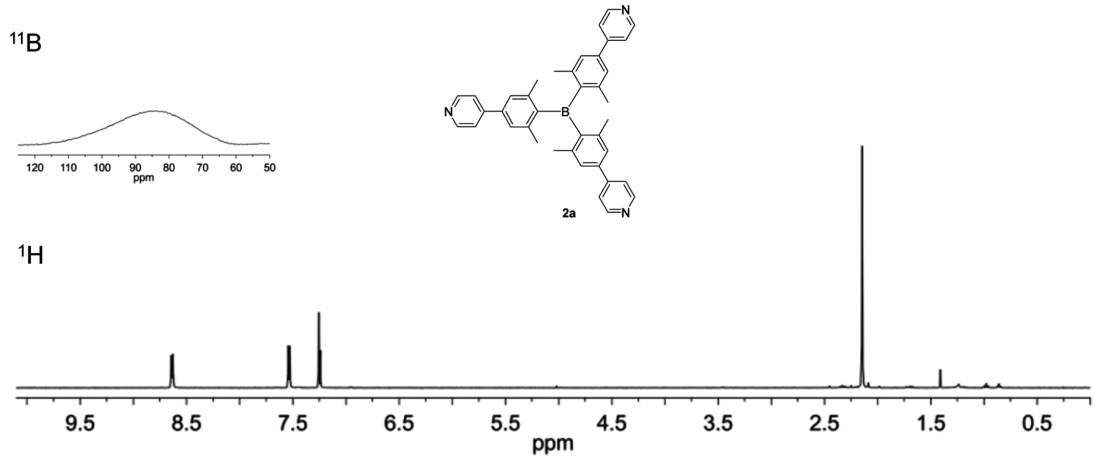

Figure S1. ^{11}B (top) and ^{1}H (bottom) NMR spectra of **2a**.

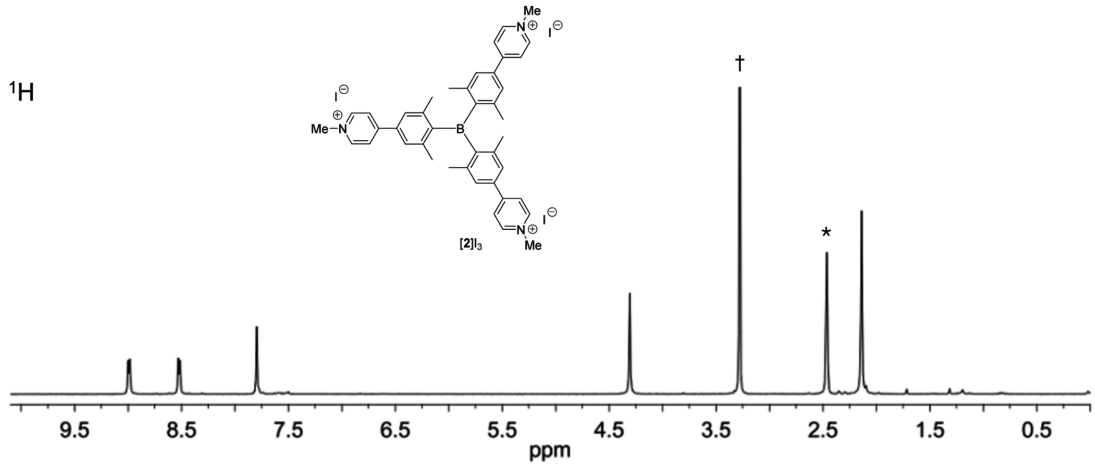

Figure S2. ^{1}H NMR spectrum of [**2**]I (∗ from DMSO-d_6 and † from H_2O).