

The Intramolecular Hydrogen Bonded-Halogen Bond: A New Strategy for Preorganization and Enhanced Binding

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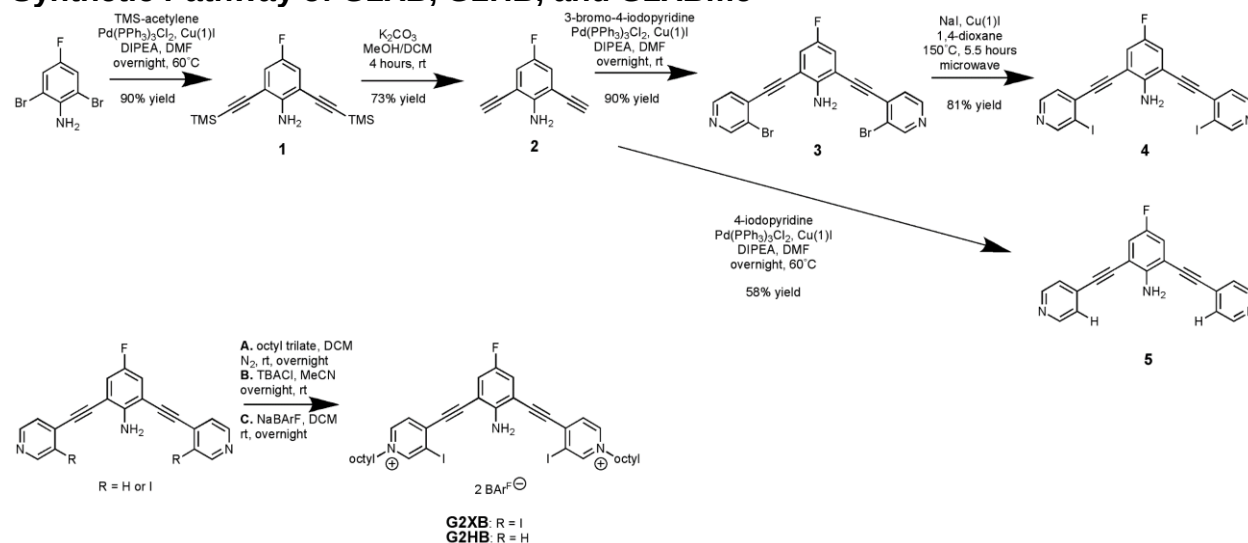
General:

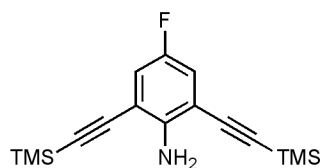
All materials were obtained from Sigma-Aldrich, Acros, TCI-America and Strem Chemicals and used without further purification. Standard Schlenk line and air-free techniques were employed for these reactions. Preparatory HPLC separations were conducted with a Teledyne Isco CombiFlash RF+. A Teledyne Isco RediSep RF Gold Reversed-phase C18 column was utilized to carry out these separations. Nuclear Magnetic Resonance ^1H NMR, ^{13}C NMR and ^{19}F NMR spectra were recorded on Varian Direct Drive 500 MHz and Bruker Avance 400 MHz spectrometers. Chemical shifts (δ) expressed as ppm. For the ^{19}F NMR spectra C_6F_6 (δ -164.9 ppm) was used as an internal standard. Signal splitting patterns are indicated as s, singlet; d, doublet; t, triplet; m, multiplet, b, broad. Coupling constants (J) are given in Hz. High-resolution masses for new compounds were obtained using an Agilent 6520 Accurate-Mass Q-TOF LC/MS. Infrared spectroscopy was taken on Thermo Scientific Nicolet IS5 using Omnic 9 software.

General procedure for anion metathesis of triflate salt to chloride salt. Octylated triflate salt of **4** or **5** was dissolved in the smallest amount of acetonitrile (enough to solubilize the receptor salt but not dilute it). 2.2 equivalents of tetra-*n*-butylammonium chloride were added to the acetonitrile mixture. Red precipitate formed upon addition of TBACl, reaction was stirred overnight at room temperature. Precipitate was gravity filtered. ^1H and ^{19}F NMR showed precipitate was clean product and no further purification was needed.

Procedures for alkylation and BArF metathesis were conducted as previously reported.¹

Synthetic Pathway of G2XB, G2HB, and G2XBme





4-fluoro-2,6-bis((trimethylsilyl)ethynyl)aniline (1). An oven dried Schlenk flask was charged with 2,6-dibromo-4-fluoroaniline (4.9787 g, 18.51 mmol), then vacuumed and backfilled with dry N₂ gas (3x). Bis(triphenylphosphine)palladium(II) dichloride (0.778 g, 1.10 mmol) was added, vacuumed and backfilled with dry N₂ (3x). Copper (I) iodide (0.354 g, 1.86 mmol) was added, vacuumed and backfilled with dry N₂ (3x). The dry reagents were dissolved in 150 mL dry dimethylformamide (DMF). N,N-diisopropylamine (16 mL, 91.85 mmol) and TMS-acetylene (6.65 mL, 46.56 mmol) were added to the DMF solution. The flask was carefully vacuumed and backfilled with dry N₂ (3x). The dark brown solution stirred overnight at 60°C. The reaction mixture was first run through a silica plug with a hexane/ethyl acetate solvent mixture (50:50) to remove any excess salts and catalysts. Subsequent removal of DMF, hexanes and ethyl acetate by roto-evaporation left a brown solid that was purified by column chromatography (gradient column of pure hexanes to 5% EtOAc/95% Hexanes) to afford **1** (5.04 g, 16.6 mmol, 90%) as a golden yellow colored oil. ¹H (400 MHz, CDCl₃, 25°C): 6.9916-6.9697 (2H, d, *J* = 8.76 Hz), 4.6717 (2H, s), 0.2598 (18H, s). ¹³C (125.7 MHz, CDCl₃, 25°C): 154.7221-152.8471 (d, *J* = 235.7 Hz), 146.8236, 119.3367 (d, *J* = 23.9 Hz), 108.0455 (d, *J* = 9.7 Hz), 101.5135, 100.2913, 0.1138. ¹⁹F (470.6 MHz, CDCl₃, 25°C): -130.7549 (1F, t, *J* = 8.73 Hz). HRMS (ESI pos) *m/z*: 304.1353 (M⁺+1, 100%); C₁₆H₂₃FN₂Si₂⁺+1 (304.1377).

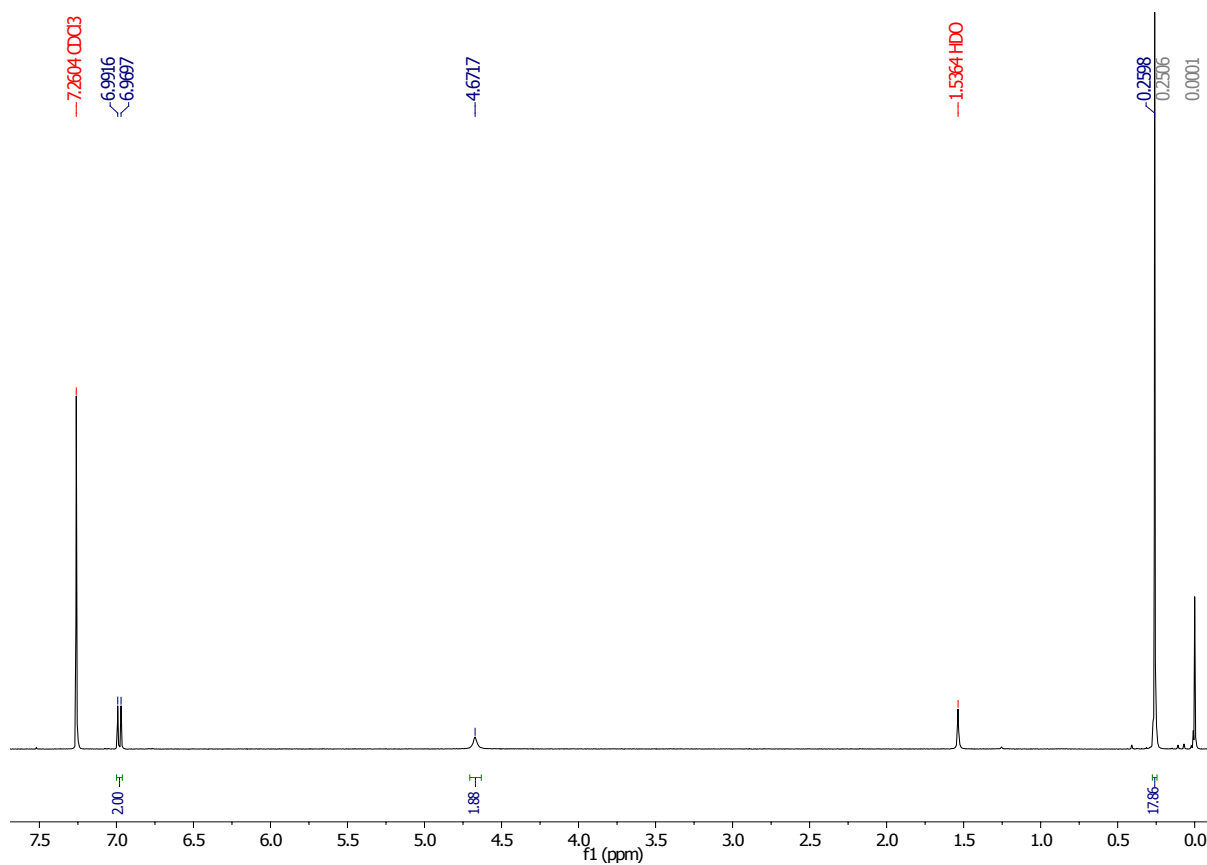


Figure S1. ^1H NMR of spectrum of **1** (CDCl_3 , 25°C , 400 MHz).

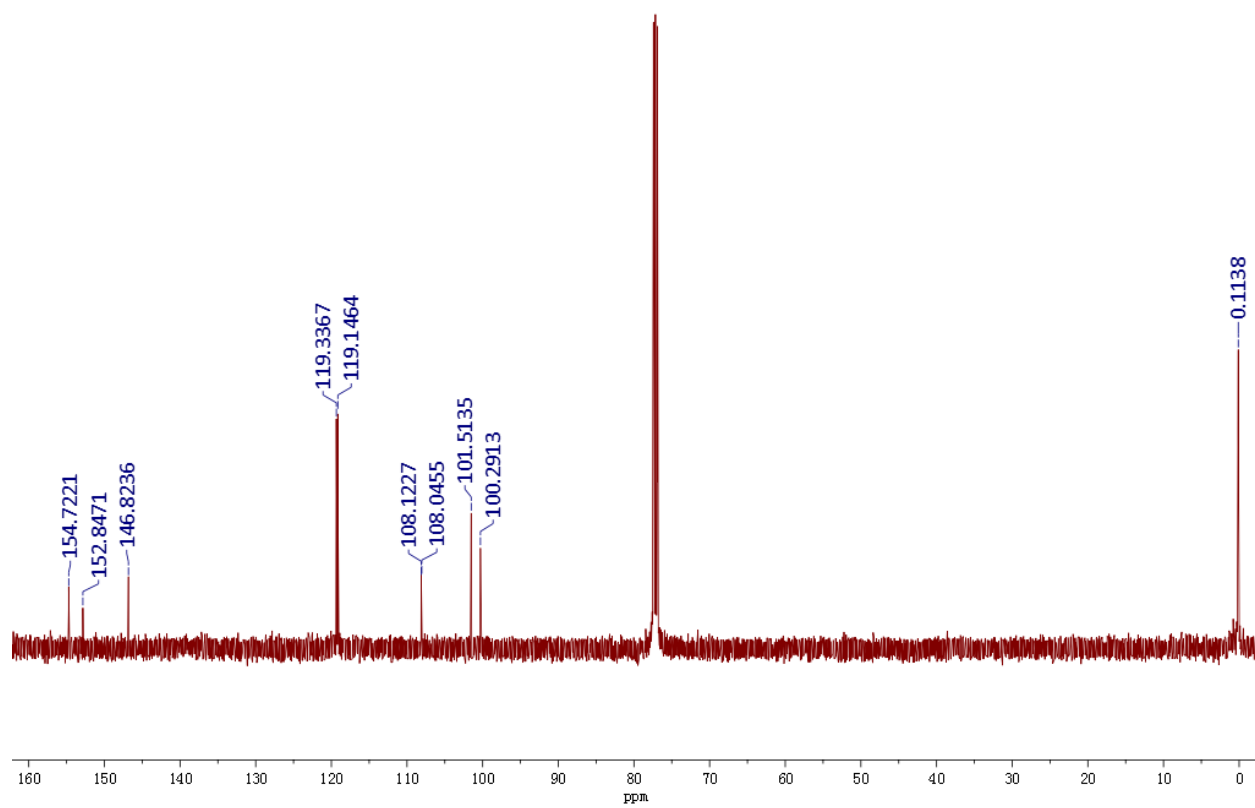


Figure S2. ^{13}C NMR of spectrum of **1** (CDCl_3 , 25°C , 125.7 MHz).

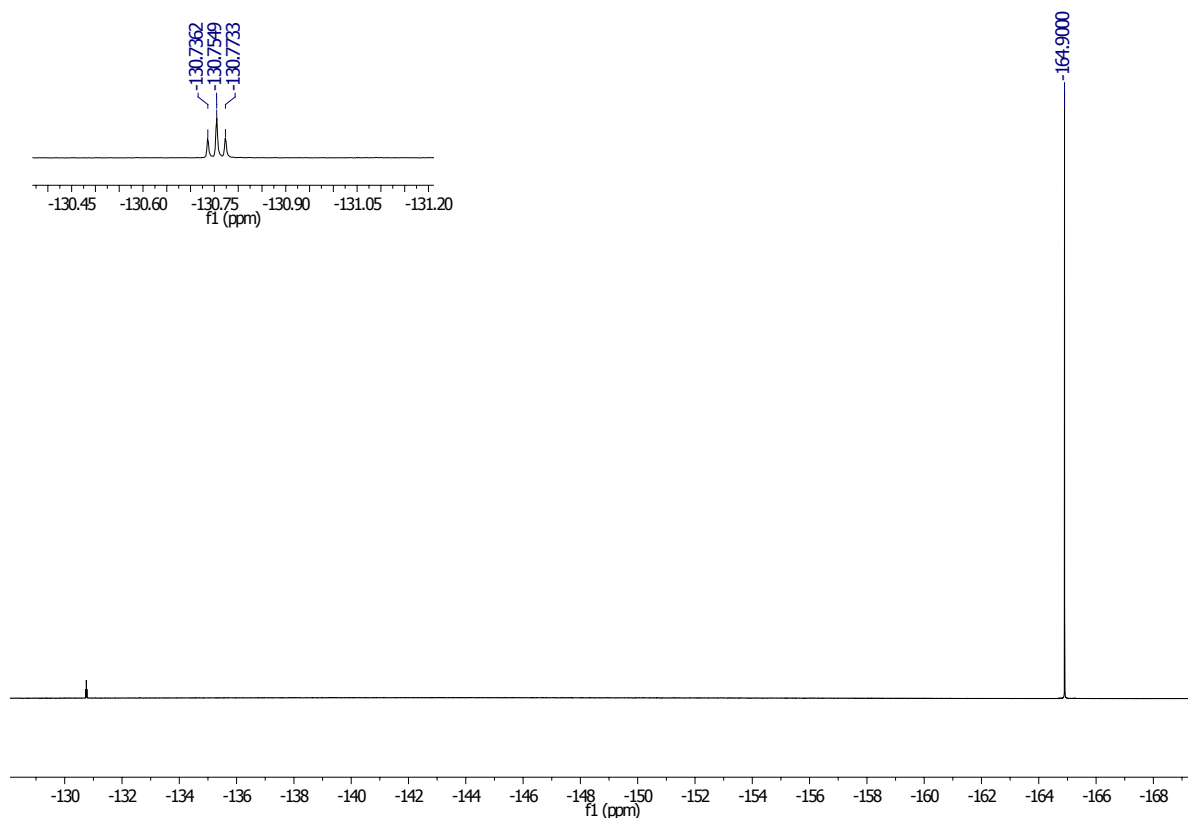
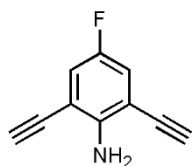


Figure S3. ^{19}F NMR of spectrum of **1** (CDCl_3 , 25°C , 470.6 MHz).



2,6-bisethynyl-4-fluoroaniline (2). **1** (1.59 g, 5.24 mmol) was dissolved in 15 mL methanol and 15 mL DCM in a 250 mL round bottom flask. Potassium carbonate (1.85 g, 13.11 mmol) was added to the organic mixture. The reaction stirred vigorously for 4 hours at room temperature and reaction progress was checked via TLC. If the reaction was not finished, it was stirred overnight. When the reaction came to completion, water was added to quench the reaction. The crude product was extracted with ethyl acetate, dried over magnesium sulfate and vacuum filtered. The organic mixture was reduced under vacuum and crude product remained a brown solid. The clean yellow solid **2** (0.610 g, 73 % yield) was obtained by column chromatography (10% DCM/90 % Hexanes). ^1H (400 MHz, CDCl_3 , 25°C): 7.0602-7.0387 (2H, d, J = 8.6 Hz), 4.7013 (2H, s), 3.4343 (2H, s). ^{13}C (125.7 Hz, CDCl_3 , 25°C): 154.6664-152.7916 (d, J = 235.7 Hz),

147.2792, 120.1869 (d, $J = 24.1$ Hz), 107.0369 (d, $J = 9.8$ Hz), 83.8922, 79.2389. ^{19}F (470.6 MHz, CDCl_3 , 25°C): -130.5275 (1F, t, $J = 8.66$ Hz). HRMS (ESI pos) m/z : 160.0563 ($\text{M}^+ + 1$, 100%); $\text{C}_{10}\text{H}_7\text{FN}^+ + 1$ (160.0563).

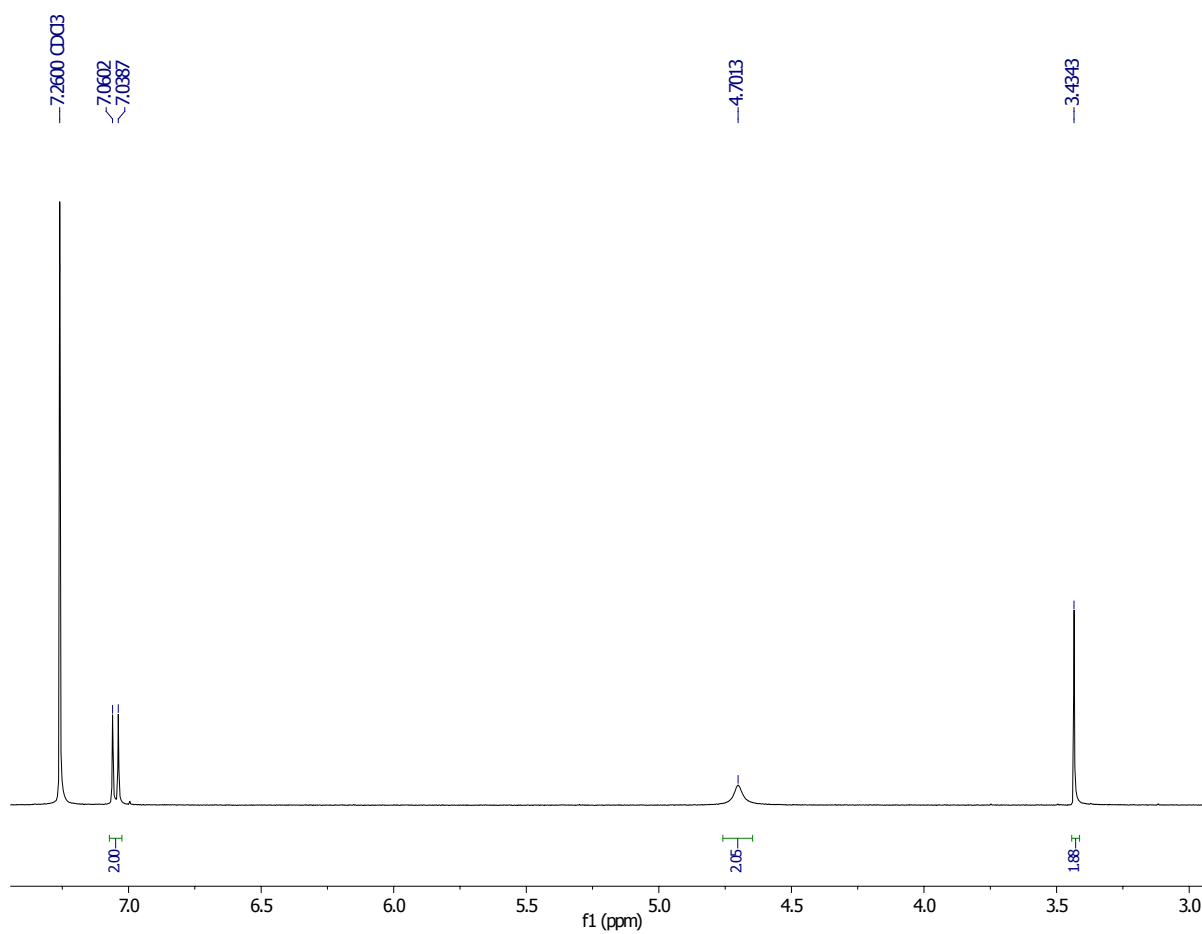


Figure S4. ^1H NMR of spectrum of **2** (CDCl_3 , 25°C, 400 MHz).

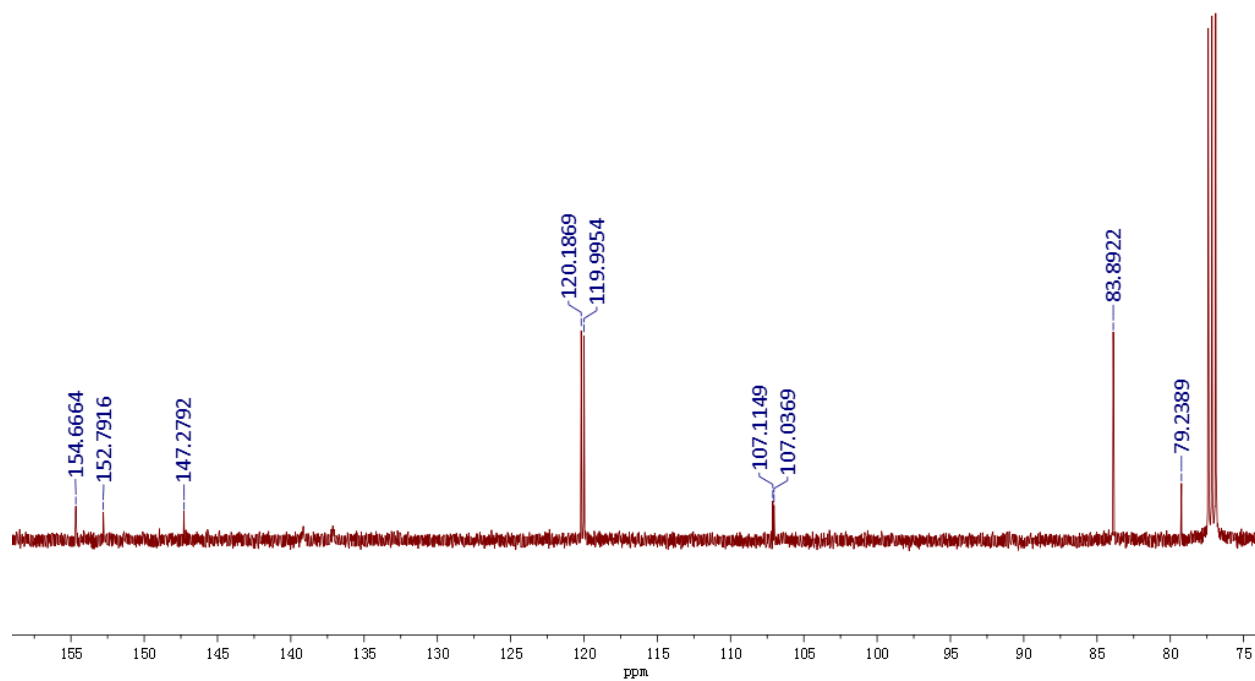


Figure S5. ^{13}C NMR of spectrum of **2** (CDCl_3 , 25°C , 125.7 MHz).

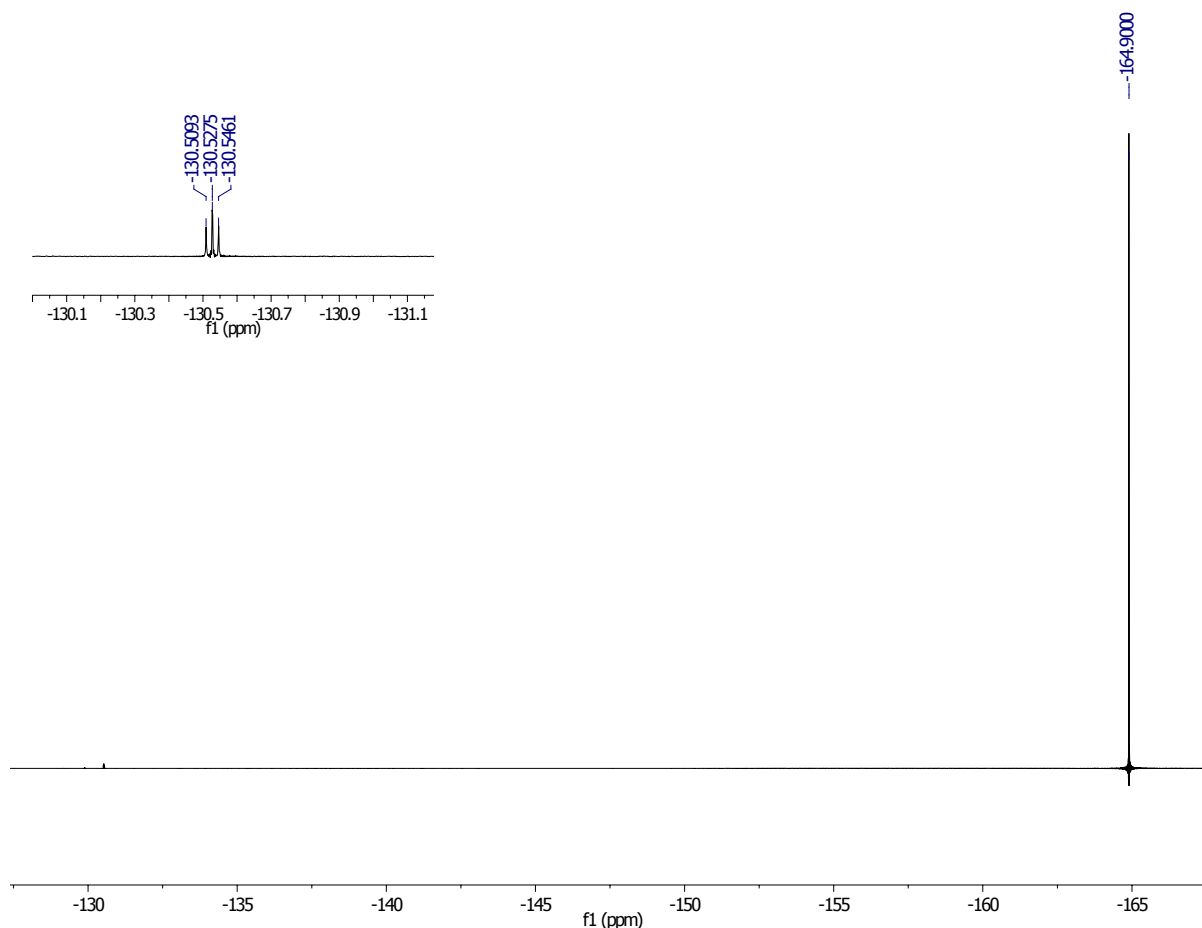
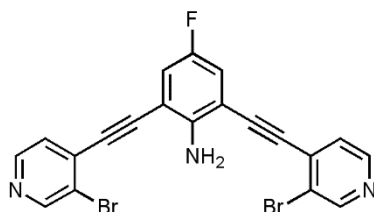


Figure S6. ^{19}F NMR of spectrum of **2** (CDCl_3 , 25°C , 470.6 MHz).



2,6-bis(4-ethynyl-3-bromopyridinyl)-4-fluoroaniline (3). An oven dried Schlenk flask was charged with **2** (0.300 g, 1.88 mmol) and 4-bromo-3-iodopyridine (1.125 g, 4.71 mmol) then vacuumed and backfilled with dry N_2 gas (3x). Bis(triphenylphosphine)palladium (II) dichloride (0.0793 g, 0.113 mmol) was added, vacuumed and backfilled with dry N_2 (3x). Copper (I) iodide (0.035 g, 0.188 mmol) was added, vacuumed and backfilled with dry N_2 (3x). The dry reagents were dissolved in 60 mL dry DMF. *N,N*-diisopropylamine (1.6 mL, 9.4 mmol) was added to the DMF solution. The flask was carefully vacuumed and backfilled with dry N_2 (3x). The dark brown solution stirred overnight at room temperature. The reaction mixture was first run through a silica plug with a hexane/ethyl acetate solvent mixture (50:50) to remove any excess salts and catalysts. Subsequent removal of DMF, hexanes and ethyl acetate by roto-evaporation left and

brown solid that was purified by column chromatography (gradient from 30% EtOAc/70% Hexanes to 75% EtOAc/25% Hexanes) to afford **3** (5.04 g, 16.6 mmol, 90%) as a bright yellow solid. ^1H (400 MHz, CDCl_3 , 25°C): 8.8199 (2H, s), 8.5531-8.5406 (2H, d, $J = 5$ Hz), 7.4405-7.4280 (2H, d, $J = 5$ Hz), 7.2255-7.2045 (2H, d, $J = 8.4$ Hz), 5.2456 (2H, s). ^{13}C (125.7 MHz, CDCl_3 , 25°C): 155.42, 153.07-152.16 (d, $J = 114.4$ Hz), 148.43, 133.02, 132.69, 126.81, 123.06, 121.46 (d, $J = 30.2$ Hz), 107.77 (d, $J = 43.0$ Hz), 94.45, 92.76. ^{19}F (470.6 MHz, CDCl_3 , 25°C): -129.9064 (1F, t, $J = 8.35$ Hz). HRMS (ESI pos) m/z : 471.9283 ($\text{M}^+ + 1$, 100%); $\text{C}_{20}\text{H}_{11}\text{Br}_2\text{FN}_3^+ + 1$ (471.9350).

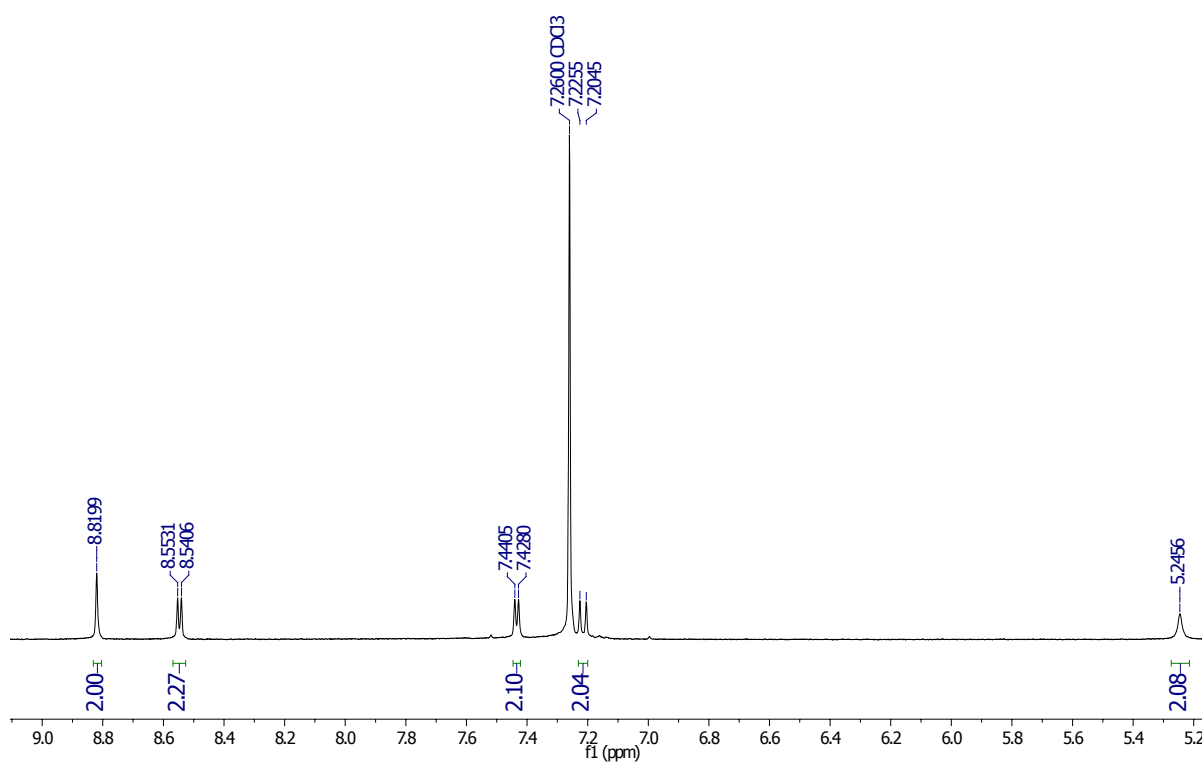


Figure S7. ^1H NMR of spectrum of **3** (CDCl_3 , 25°C , 400 MHz).

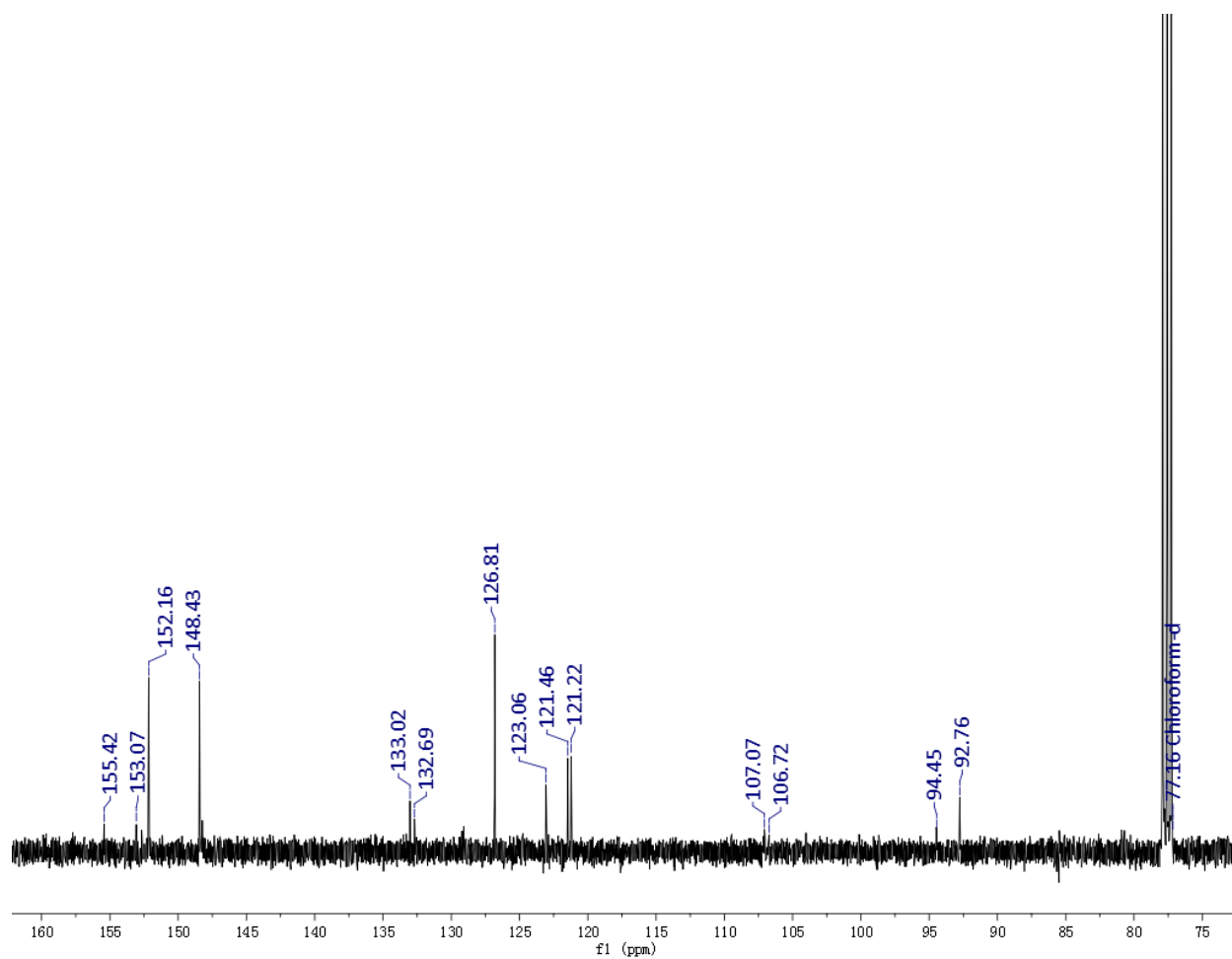


Figure S8. ^{13}C NMR of spectrum of **3** (CDCl_3 , 25°C , 125.7 MHz).

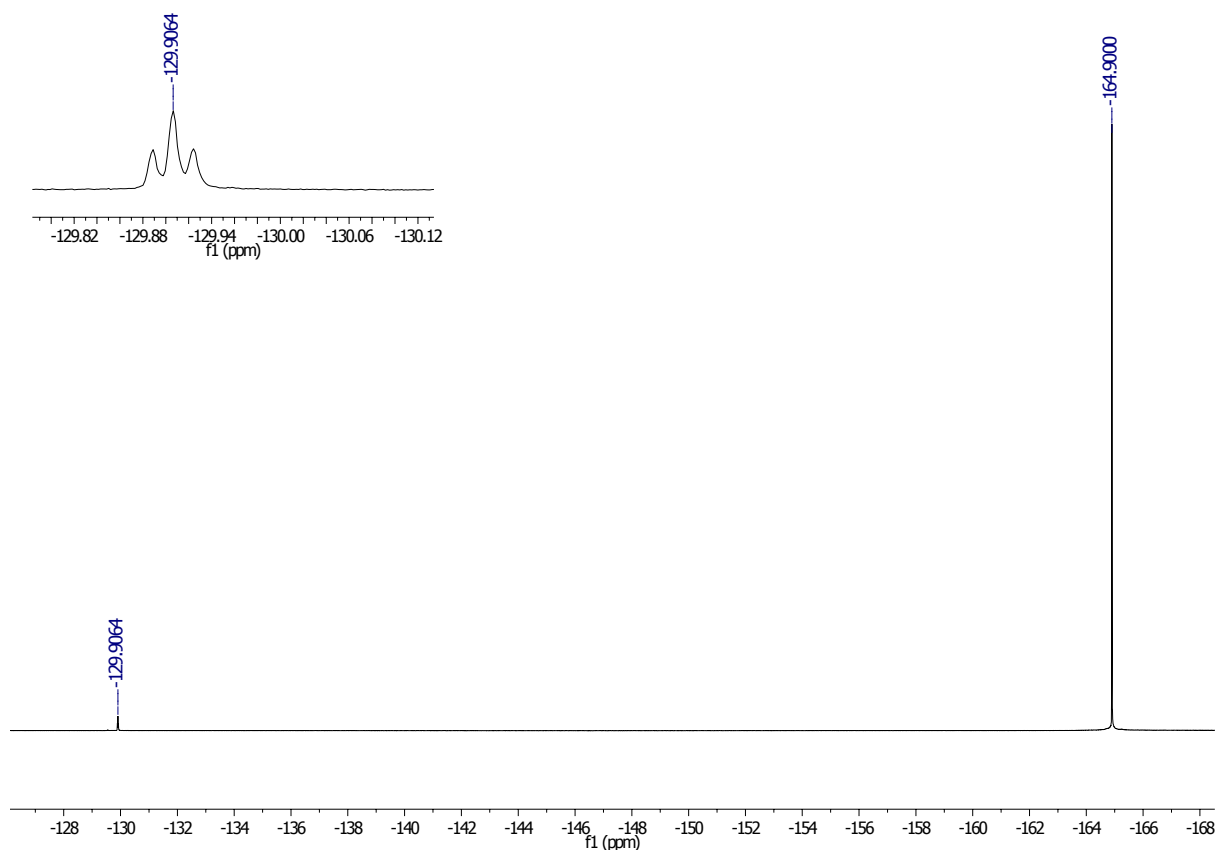
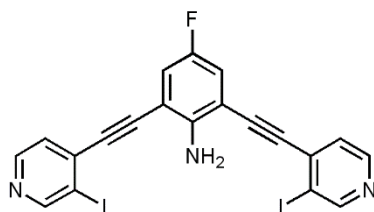


Figure S9. ^{19}F NMR of spectrum of **3** (CDCl_3 , 25°C , 470.6 MHz).



2,6-bis(4-ethynyl-3-iodopyridinyl)-4-fluoroaniline (4). **3** (0.225 g, 0.47 mmol), copper iodide (0.009 g, 0.047 mmol), sodium iodide (0.286 g, 1.91 mmol) were added to a 10-20 mL microwave reaction vial containing a stir bar and dissolved in 13 mL 1,4-dioxane. To the vibrant yellow reaction mixture, trans-N,N'-dimethylcyclohexane-1,2-diamine (0.23 mL, 1.45 mmol) was added which turned the solution color green-brown. The microwave vial was sealed and placed in a microwave. The reaction was performed in a Biotage Initiator+ microwave reactor for 5.5 hours at 150°C . After cooling, an aliquot was run through pipet silica plug with EtOAc to remove catalysts and salts. The EtOAc crude was then ran through GCMS in order to obtain % conversion of bromines to iodines. If the reaction was unfinished, it would be submitted again at 30 min increments. When the reaction ran to completion, the crude reaction was run

through a silica plug with EtOAc. The bright yellow product (0.219 g, 0.39 mmol, 81%) was purified via column chromatography (gradient column 30% EtOAc/70% Hexanes to 70% EtOAc/30% Hexanes). ^1H (400 MHz, CDCl_3 , 25°C): 9.0073 (2H, s), 8.5603-8.5478 (2H, d, $J = 5$ Hz), 7.4334-7.4209 (2H, d, $J = 5$ Hz), 7.2380-7.21770 (2H, d, $J = 8.4$ Hz), 5.3240 (2H, s). ^{13}C (125.7 MHz, CDCl_3 , 25°C): 157.1417, 154.7946-152.9078 (d, $J = 237.2$ Hz), 148.6974, 147.7629, 136.7807, 126.3512, 120.8622 (d, $J = 24.0$ Hz), 106.7141 (d, $J = 9.7$ Hz), 98.9006, 95.5187, 92.9690. ^{19}F (470.6 MHz, CDCl_3 , 25°C): -129.8910 (1F, t, $J = 8.3$ Hz). HRMS (ESI pos) m/z : 565.9026 ($\text{M}^+ + 1$, 100%); $\text{C}_{20}\text{H}_{11}\text{F}_2\text{N}_3^+ + 1$ (565.9040).

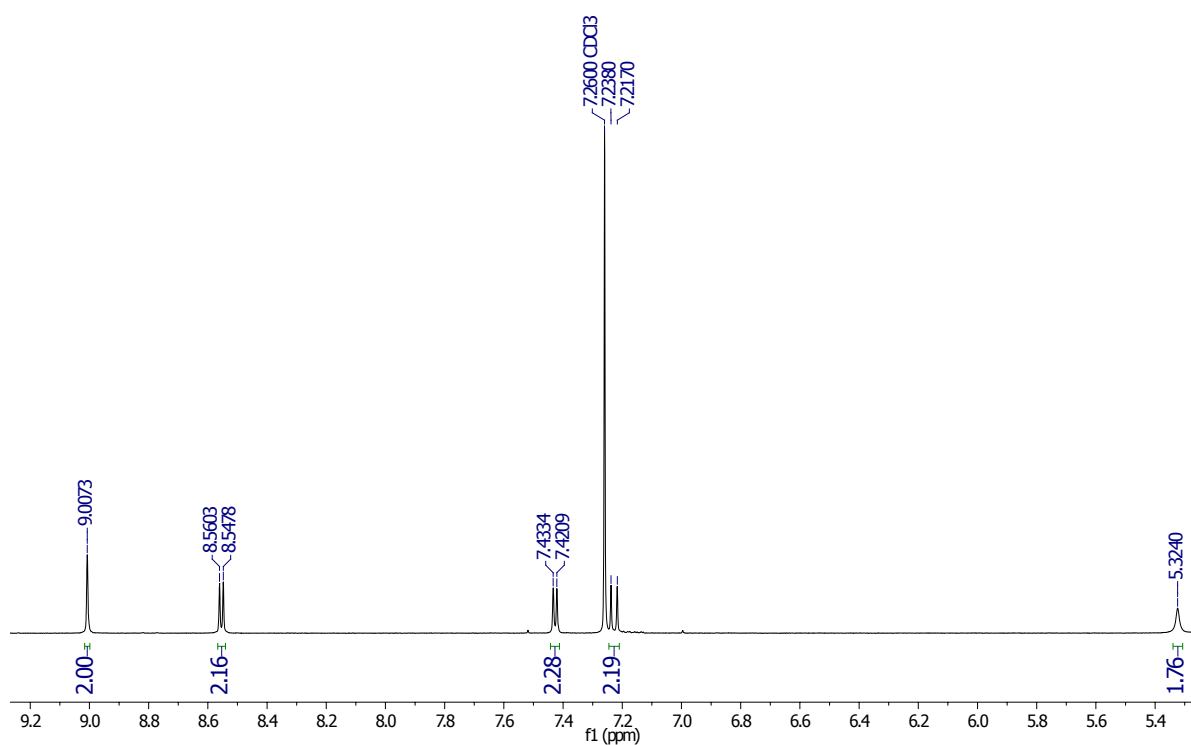


Figure S10. ^1H NMR of spectrum of **4** (CDCl_3 , 25°C , 400 MHz).

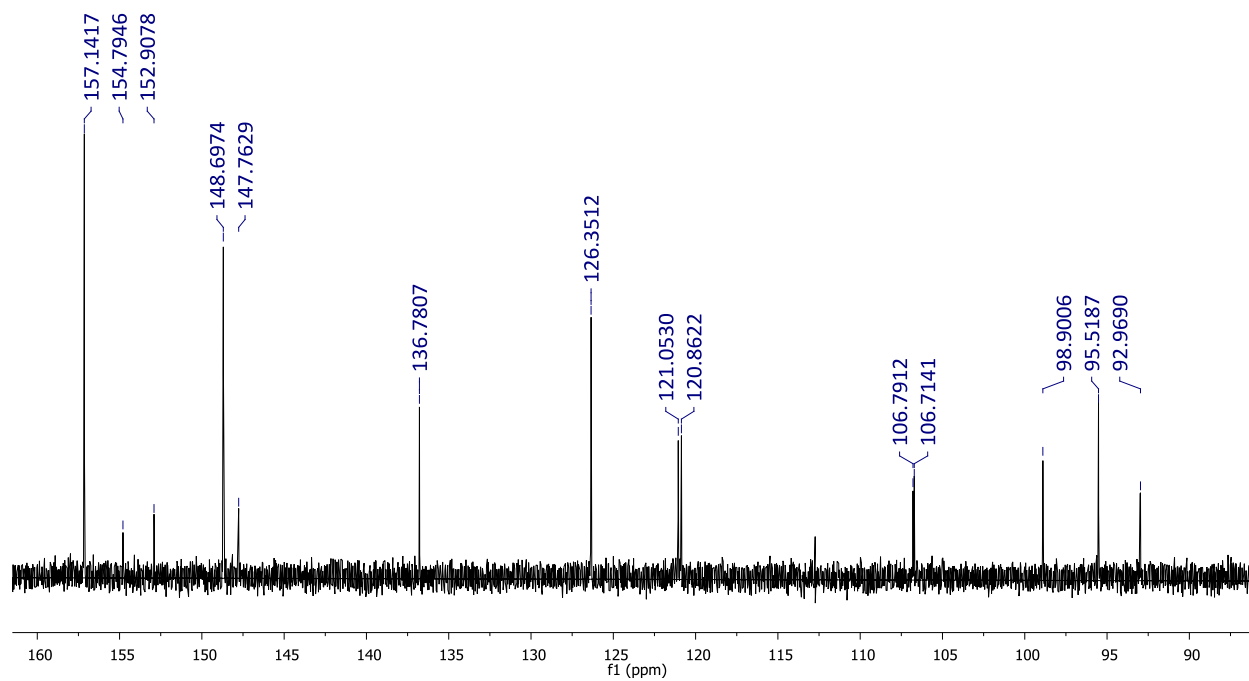


Figure S11. ¹³C NMR of spectrum of **4** (CDCl₃, 25°C, 125.7 MHz).

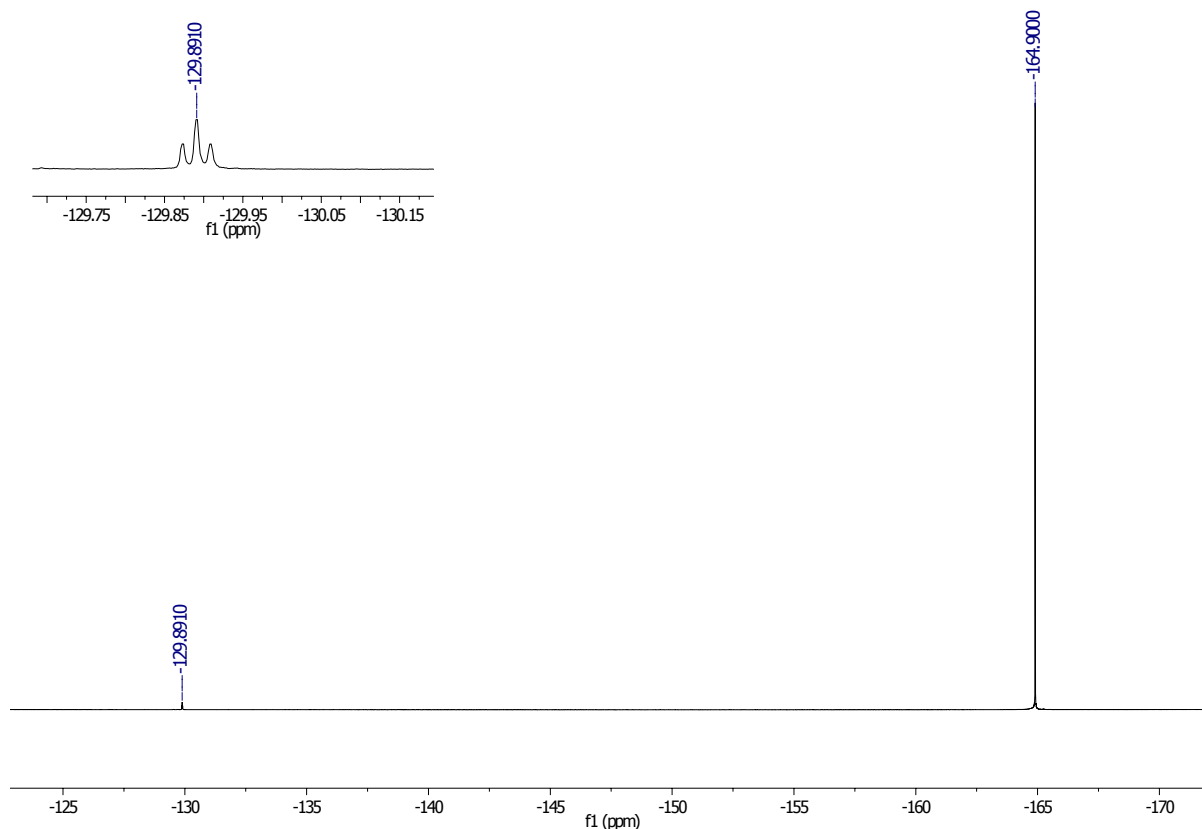
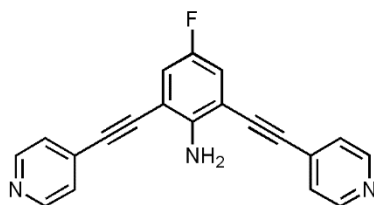


Figure S12. ^{19}F NMR of spectrum of **4** (CDCl_3 , 25°C , 470.6 MHz).



2,6-bis(4-ethynylpyridinyl)-4-fluoroaniline (5). An oven dried Schlenk flask was charged with **2** (0.85 g, 5.34 mmol) and 4-iodopyridine (2.5 g, 12.2 mmol) then vacuumed and backfilled with dry N_2 gas (3x). Bis(triphenylphosphine)palladium (II) dichloride (0.226 g, 0.342 mmol) was added, vacuumed and backfilled with dry N_2 (3x). Copper (I) iodide (0.101 g, 0.53 mmol) was added, vacuumed and backfilled with dry N_2 (3x). The dry reagents were dissolved in 40 mL dry DMF. *N,N*-diisopropylamine (4.6 mL, 26.4 mmol) was added to the DMF solution. The flask was carefully vacuumed and backfilled with dry N_2 (3x). The dark brown solution stirred overnight at 150°C . The reaction mixture was first run through a silica plug with an ethyl acetate/methanol solvent mixture (90:10) to remove any excess salts and catalysts. Subsequent removal of DMF, hexanes and ethyl acetate by roto-evaporation left a brown solid that was

purified by column chromatography (gradient from 30% EtOAc/70% Hexanes to 75% EtOAc/25% Hexanes) to afford **5** (0.96 g, 3.1 mmol, 58%) as a bright yellow solid. ^1H (500 MHz, CD_3CN , 25°C): 8.6234-8.6114 (2H, d, $J = 6$ Hz), 7.5059-7.4938 (4H, d, $J = 6.05$ Hz), 7.2422-7.2245 (2H, d, $J = 8.85$ Hz), 5.2600 (2H, s). ^{13}C (125.7 MHz, CD_3CN , 25°C): 155.3862, 151.0052 (d, $J = 6.9$ Hz), 150.9501, 148.4883, 131.3914, 126.2978, 121.2470, 121.0545 (d, $J = 24.2$ Hz), 107.8108, 107.7302 (d, $J = 10.13$ Hz), 93.8579, 89.3939. ^{19}F (470.6 MHz, CD_3CN , 25°C): -129.6846 (1F, t, $J = 8.82$ Hz). HRMS (ESI pos) m/z : 314.1094 ($\text{M}^+ + 1$, 100%); $\text{C}_{20}\text{H}_{13}\text{FN}_3^+ + 1$ (314.1107).

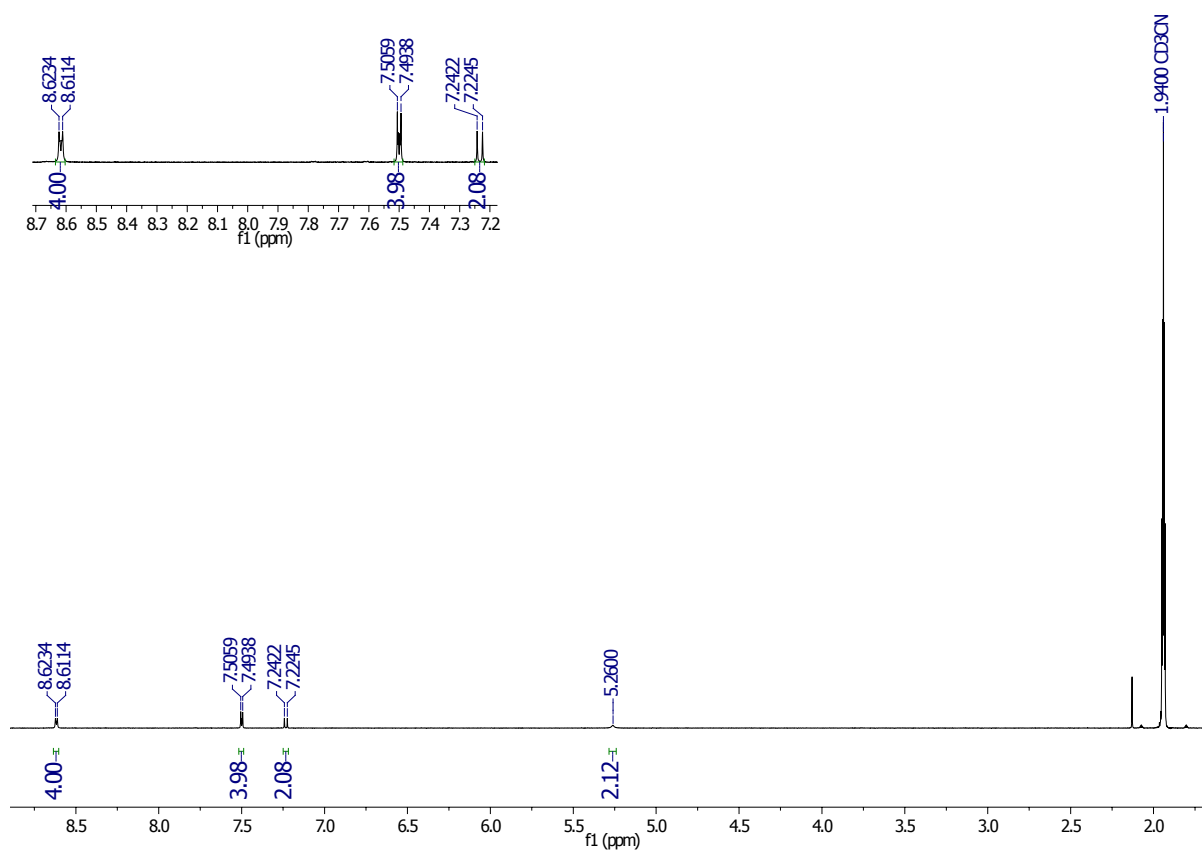


Figure S13. ^1H NMR of spectrum of **5** (CD_3CN , 25°C , 500 MHz).

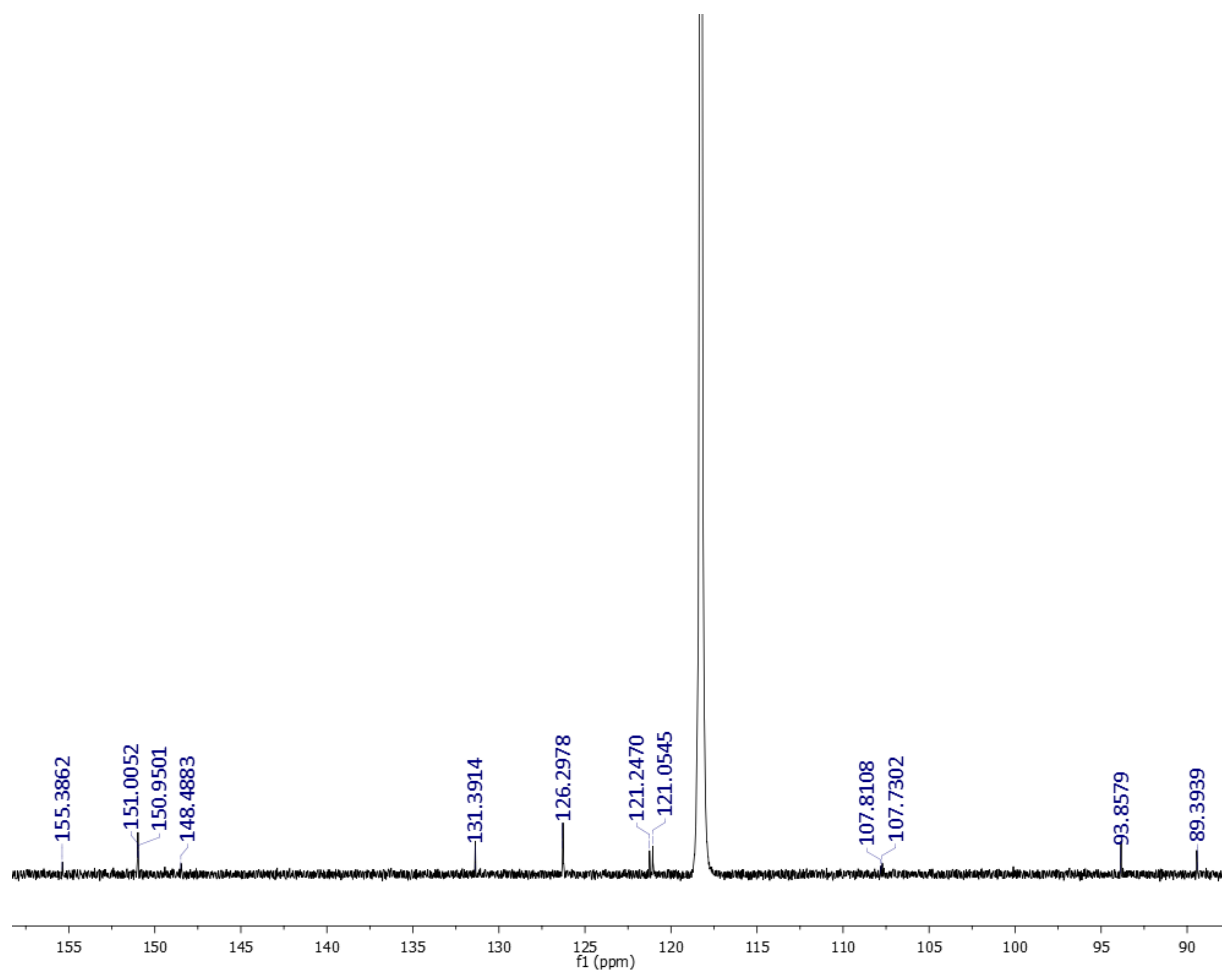


Figure S14. ^{13}C NMR of spectrum of **5** (CD_3CN , 25°C , 125.7 MHz).

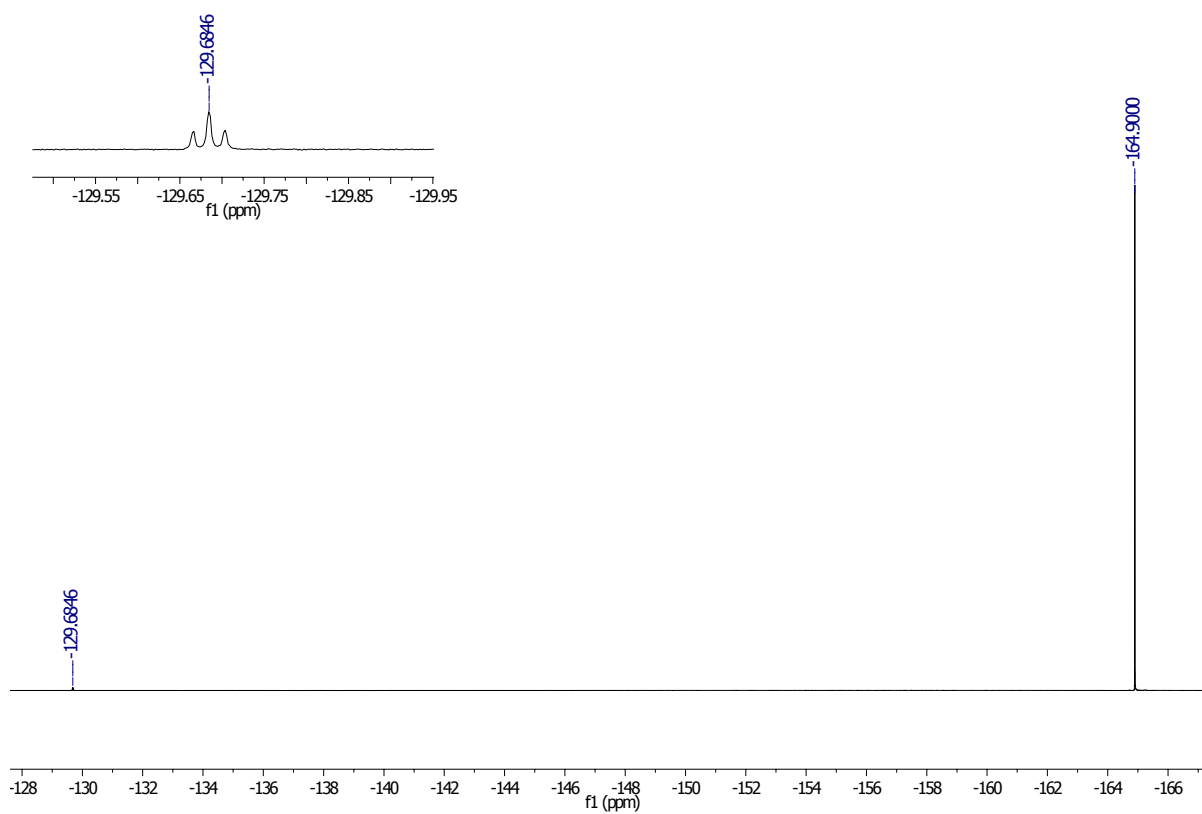
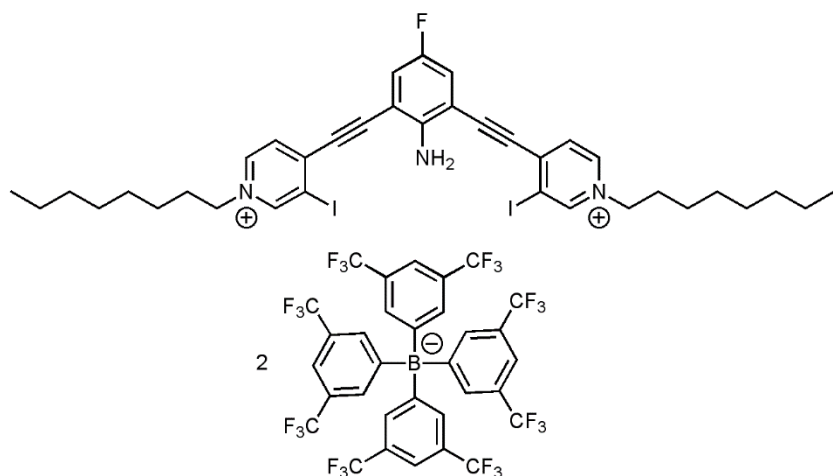


Figure S15. ^{19}F NMR of spectrum of **5** (CD_3CN , 25°C , 470.6 MHz).



G2XB (6). ^1H (500 MHz, CDCl_3 , 25°C): 8.6111 (2H, s), 8.0362-8.0211 (2H, d, $J = 7.55$ Hz), 7.6914 (16H, b), 7.6045-7.5917 (2H, d, $J = 6.54$ Hz), 7.4989 (8H, b), 7.3652-7.3500 (2H, d, $J = 7.65$ Hz), 5.2924 (2H, s), 4.2338 (4H, t, $J = 7.05$ Hz), 1.9174 (4H, b), 1.3144-1.2317 (20H, b), 0.8460 (6H, t). ^{13}C (125.7 MHz, CDCl_3 , 25°C): 162.6471-161.4581 (dd, $J = 99.95$ Hz, $J = 45.55$ Hz), 150.1248, 149.3866, 147.4292, 141.0047, 135.1731, 129.7229-128.9098 (qq, $J = 34.07$ Hz), 128.2168-121.6206 (q, $J = 272.61$ Hz), 125.5778, 125.3818, 117.9445, 106.9363, 105.1553 (d, $J = 7.41$ Hz), 99.6546, 95.5300, 63.1093, 31.7955, 31.7420, 29.0824, 28.9629, 26.3058, 22.8052, 14.2414. ^{19}F (470.6 MHz, CDCl_3 , 25°C): -126.7810 (1F, t, $J = 7.65$ Hz), -65.3734 (48F, s). HRMS (ESI pos) m/z : 395.5805 (M^{+2} , 100%), 1654.2257 ($\text{M}^+ - 1\text{BAr}^{\text{F}}$); $\text{C}_{36}\text{H}_{44}\text{F}_{12}\text{N}_3^{+2}$ (395.5814), $\text{C}_{68}\text{H}_{56}\text{BF}_{25}\text{I}_2\text{N}_3^+$ (1654.2241).

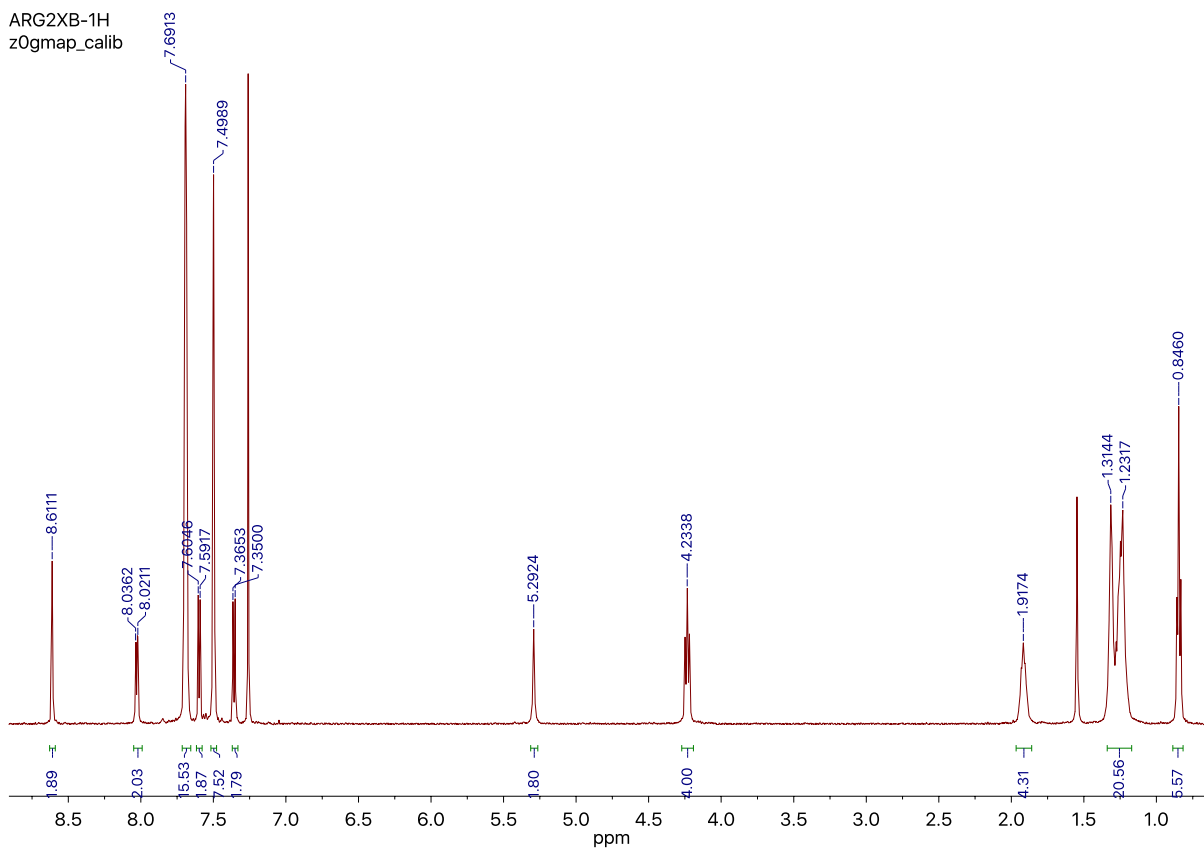


Figure S16. ^1H NMR of spectrum of **6** (CDCl_3 , 25°C , 500 MHz).

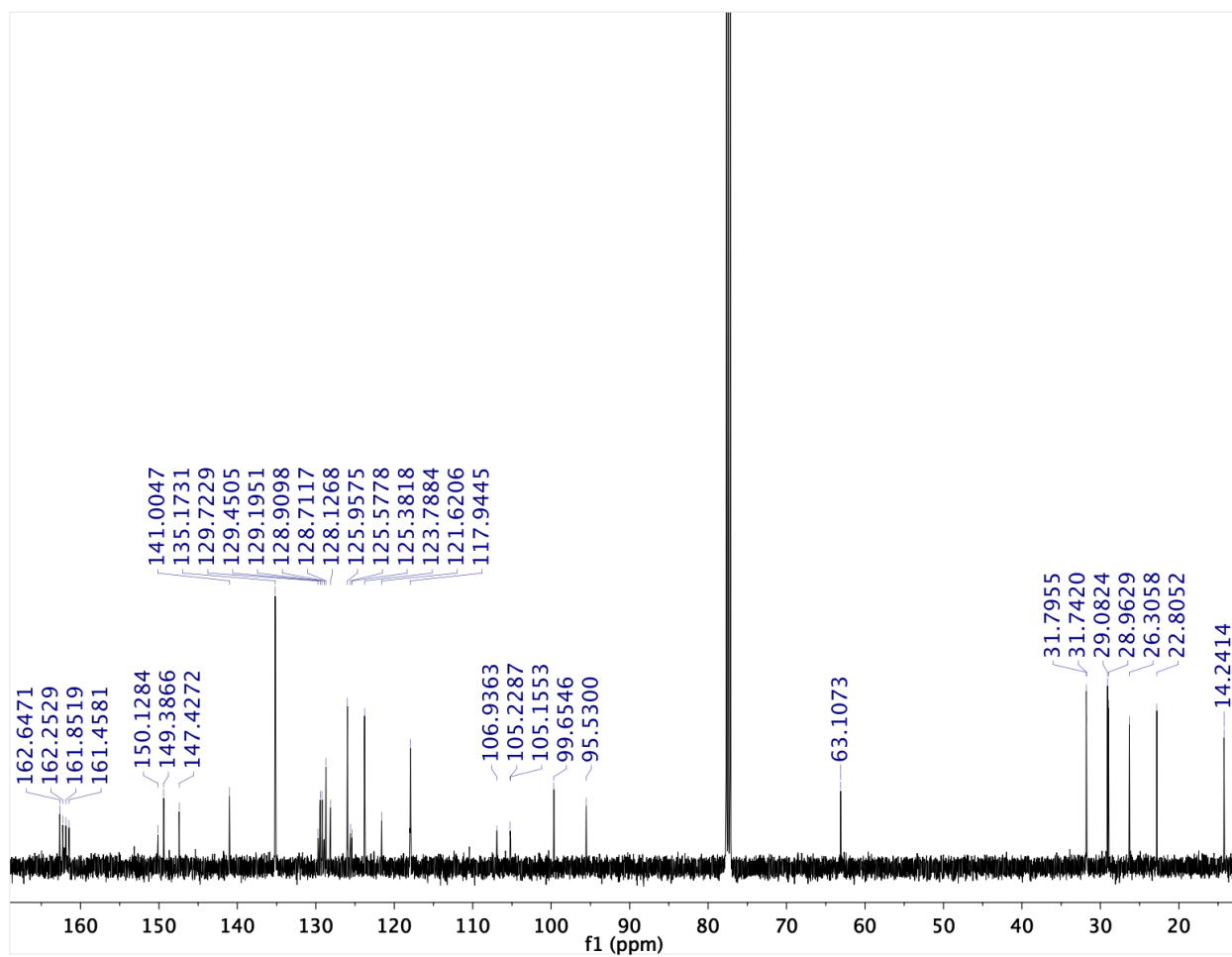


Figure S17. ¹³C NMR of spectrum of **6** (CDCl₃, 25°C, 125.7 MHz).

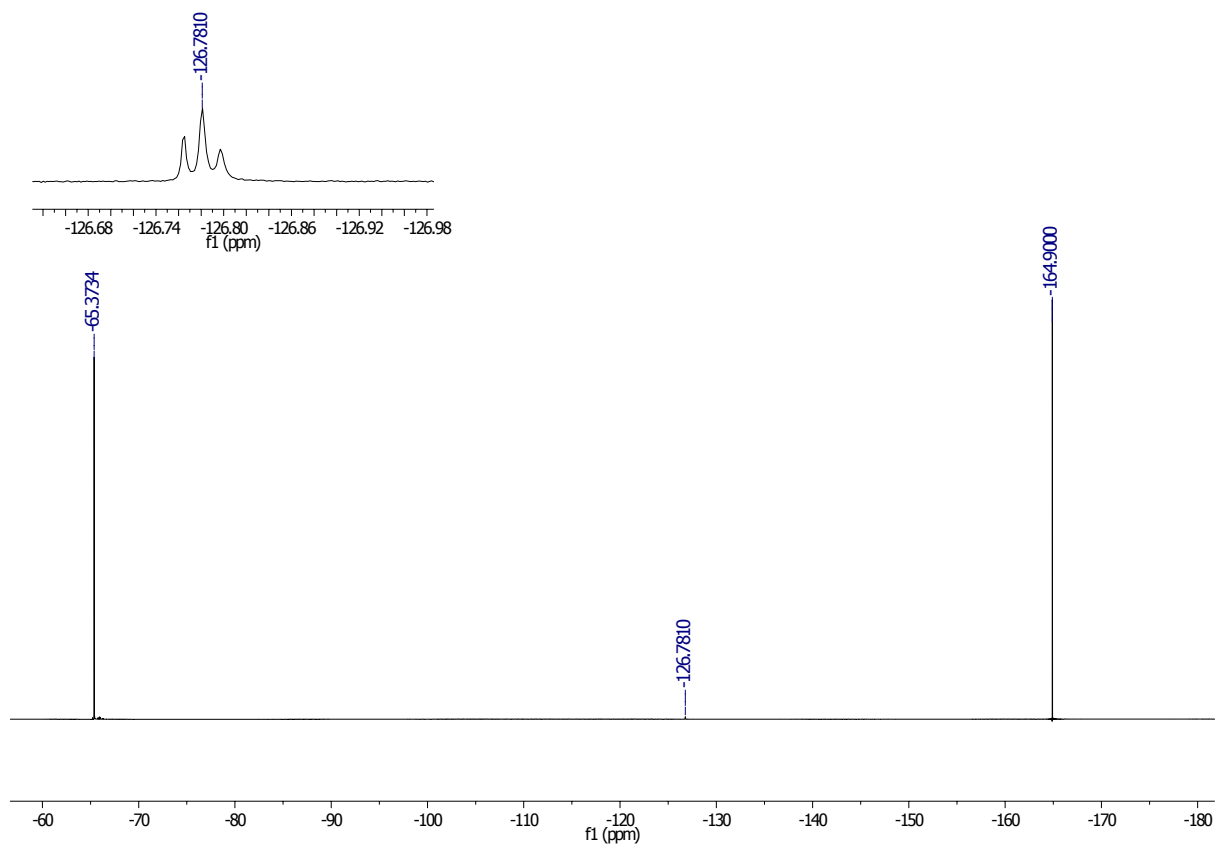
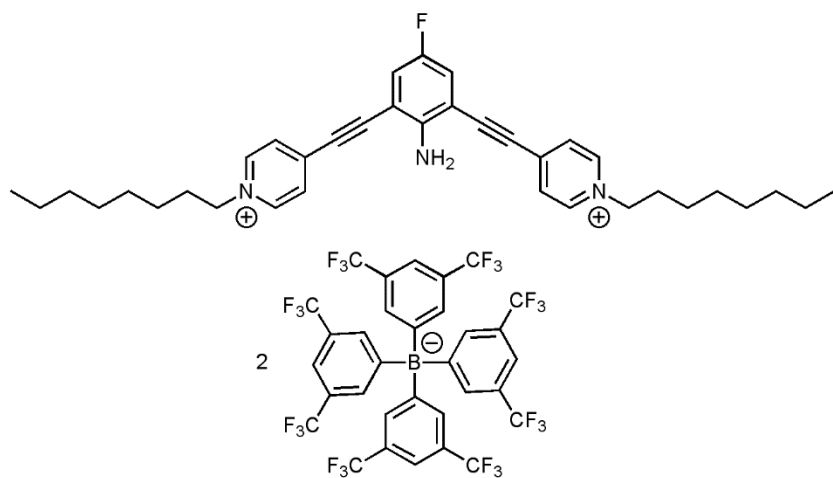


Figure S18. ^{19}F NMR of spectrum of **6** (CDCl_3 , 25°C , 470.6 MHz).



G2HB (7). ^1H (500 MHz, 60:40 $\text{CD}_3\text{NO}_2:\text{CDCl}_3$, 25°C): 8.5068-8.4937 (4H, d, $J = 8.5$ Hz), 7.9210-7.9076 (4H, d, $J = 7.9$ Hz), 7.5526 (16H, b), 7.4020 (8H, b), 7.2078-7.1910 (2H, d, $J = 7.2$ Hz), 4.4120-4.3824 (4H, t, $J = 4.4$ Hz), 1.8655 (4H, b), 1.1935 (20H, b), 0.6813 (6H, t). ^{13}C (125.7 MHz, CDCl_3 , 25°C): 162.3783-161.1915 (dd, $J = 99.24$ Hz, $J = 49.59$ Hz), 151.0880, 148.6799, 142.4386, 141.5833, 134.8523, 129.6429, 129.4794-128.7591 (qq, $J = 29.85$ Hz), 127.8469-121.4307 (q, $J = 272.61$ Hz), 124.5287, 124.3342, 117.6843, 117.6541, 105.0992-105.0244 (d, $J = 7.55$ Hz), 102.6996, 91.0861, 62.9674, 31.5562, 31.4401, 28.8630, 28.7388, 26.0454, 22.5690. ^{19}F (470.6 MHz, CDCl_3 , 25°C): -126.9895 (t, $J = 7.81$ Hz, 1F), -65.4280 (48F, s). HRMS (ESI pos) m/z : 269.6838 (M^{+2} , 100%), 1402.4325 ($\text{M}^{+}-1\text{BAr}^{\text{F}}$); $\text{C}_{36}\text{H}_{44}\text{F}_2\text{N}_3^{+2}$ (269.6840), $\text{C}_{68}\text{H}_{56}\text{BF}_{25}\text{I}_2\text{N}_3^{+}$ (1402.4325).

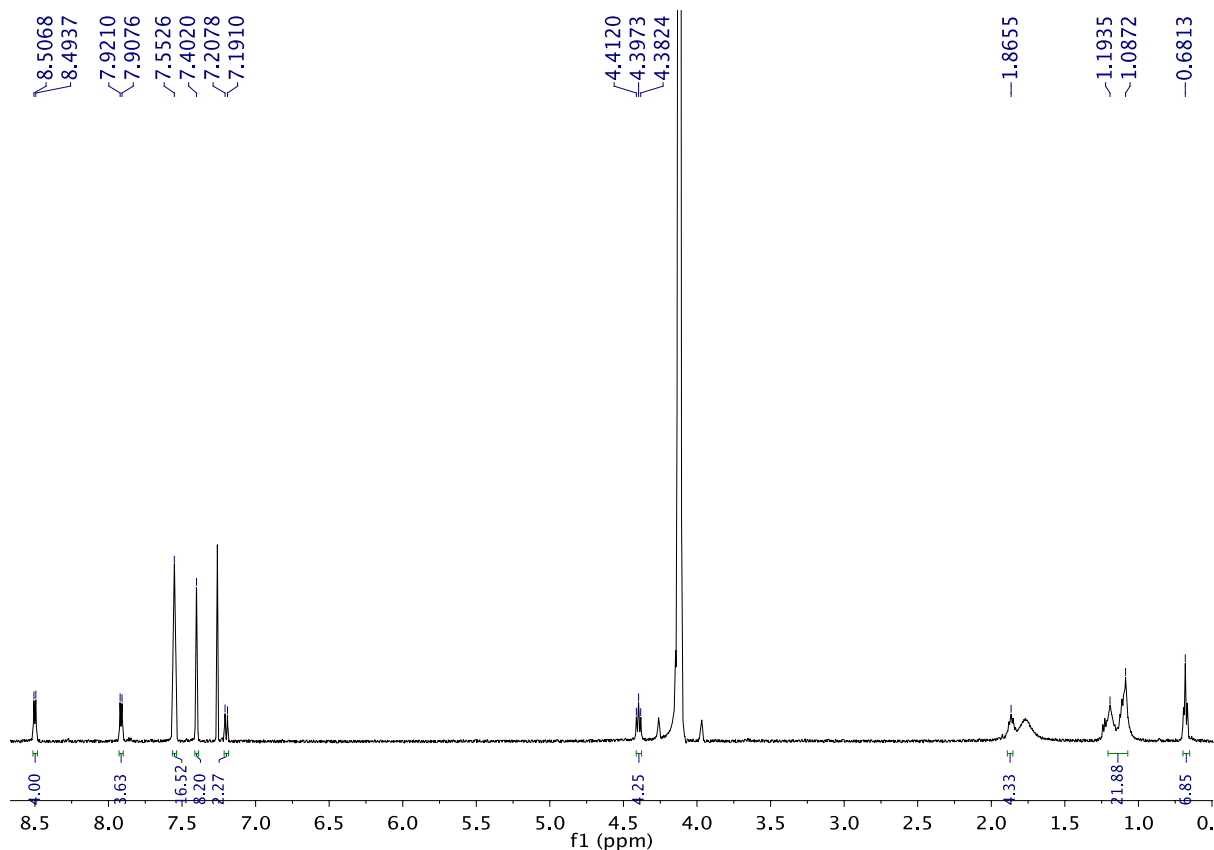


Figure S19. ^1H NMR of spectrum of **7** (CDCl_3 , 25°C , 500 MHz).

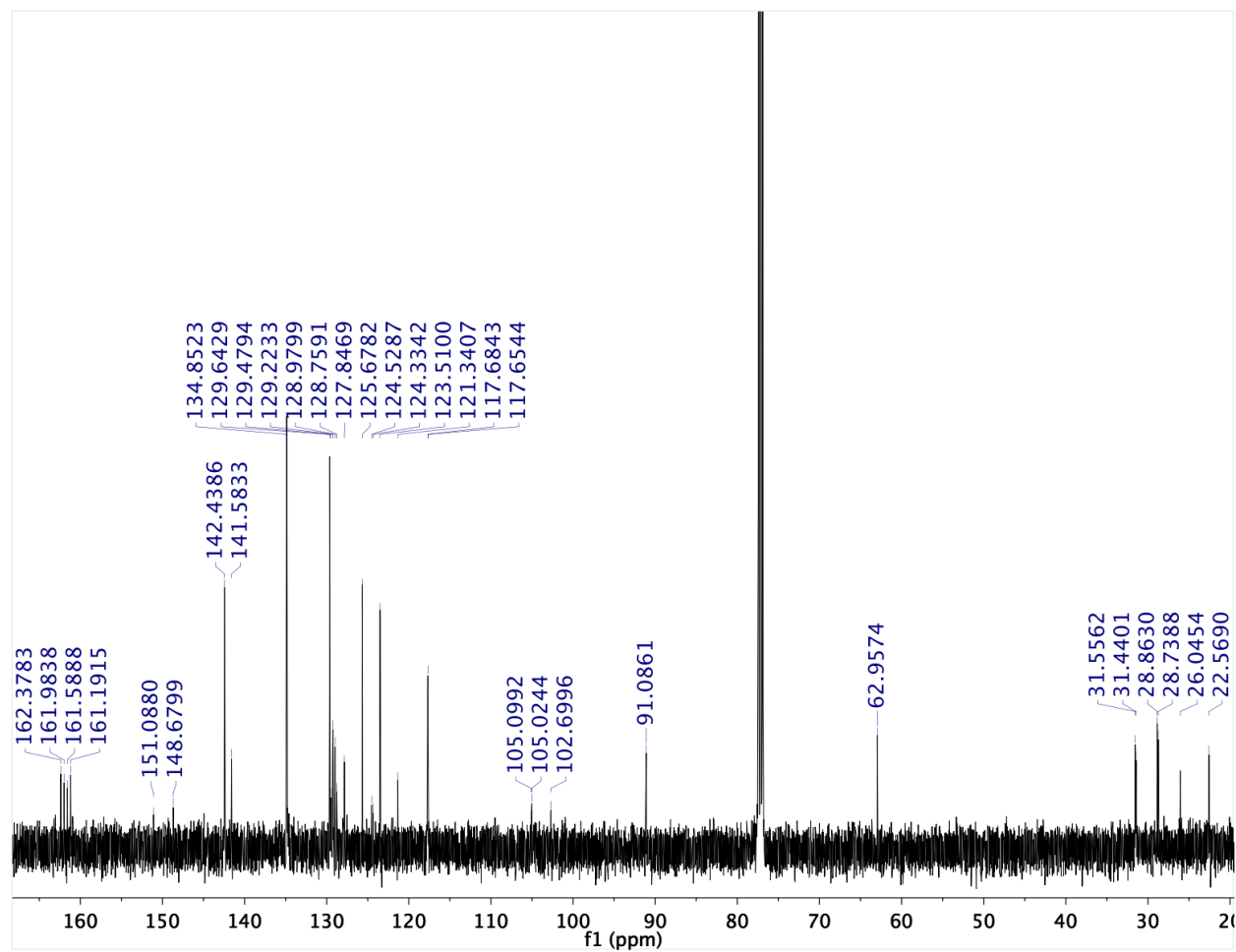


Figure S20. ¹³C NMR of spectrum of **7** (CDCl₃, 25°C, 125.7 MHz).

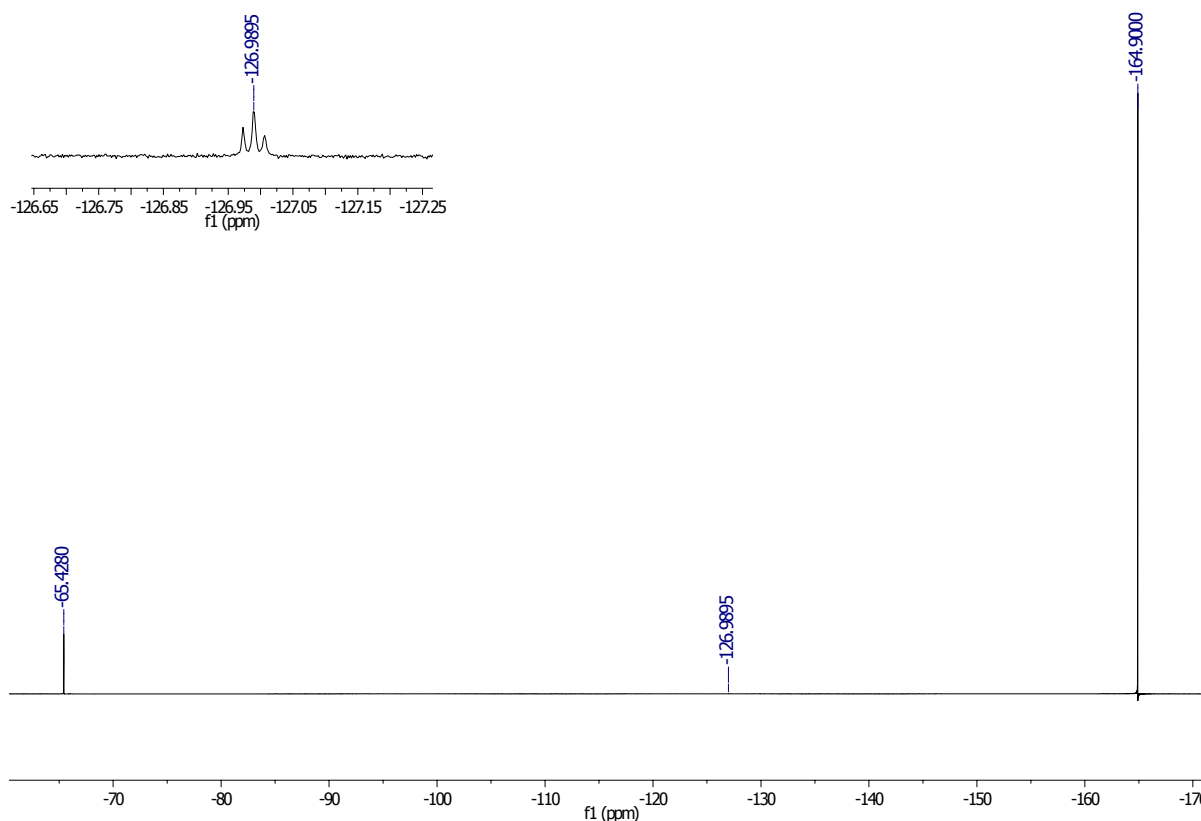


Figure S21. ^1H NMR of spectrum of **7** (CDCl_3 , 25°C , 470.6 MHz).

NMR Titrations

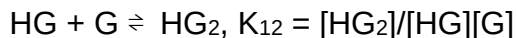
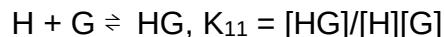
All experiments were performed on a Varian Drive Direct 500 MHz NMR Spectrometer. CD_3NO_2 was used with no further purification. CDCl_3 was dried over 3 Å molecular sieves. TBA^+ salts (Cl^- , Br^- , I^-) was dried under vacuum and stored in a desiccator.

^1H NMR Titrations

General:

Stock solutions of **G2XB** (1.504 ± 0.012 mM), **G2HB** (1.511 ± 0.011 mM), **G1XB** (1.503 ± 0.012 mM) and **G1HB** (1.521 ± 0.013 mM) were prepared in 1.660 mL of $\text{CD}_3\text{NO}_2/\text{CDCl}_3$ (3:2 v/v). 0.500 mL aliquots from each stock solution were syringed into three separate NMR tubes with screw caps and septa. The stock solution of each host was then used to make three guest solutions. After obtaining free-host spectra of **G2XB**, **G2HB**, **G1XB** and **G1HB**, aliquots of corresponding guest solution were added to their respective NMR tubes. Spectra were obtained after each addition (20x). A constant host concentration was maintained, while TBA^+ salt concentrations gradually increased throughout the

titration (see data below). Intuitions of stoichiometric displacement led to the stepwise anion exchange model:



A simple 1:1 model, dimerization, and higher order binding were ruled out due to the emergence of an obvious pattern in residuals, unrealistic assigned shifts, poor convergence, and/or larger standard deviations. HypNMR 2008 was used to refine the isothermal fits of multiple signals simultaneously.

	G2XB		G1XB		G2HB		G1HB	
	K_{11} (M^{-1})	K_{12} (M^{-1})	K_{11} (M^{-1})	K_{12} (M^{-1})	K_{11} (M^{-1})	K_{12} (M^{-1})	K_{11} (M^{-1})	K_{12} (M^{-1})
Cl⁻	23652	25	2629	37	2503	47	9043	38
Br⁻	32888	35	4688	32	2108	44	1145	38
I⁻	36943	28	4384	28	1753	44	1031	33

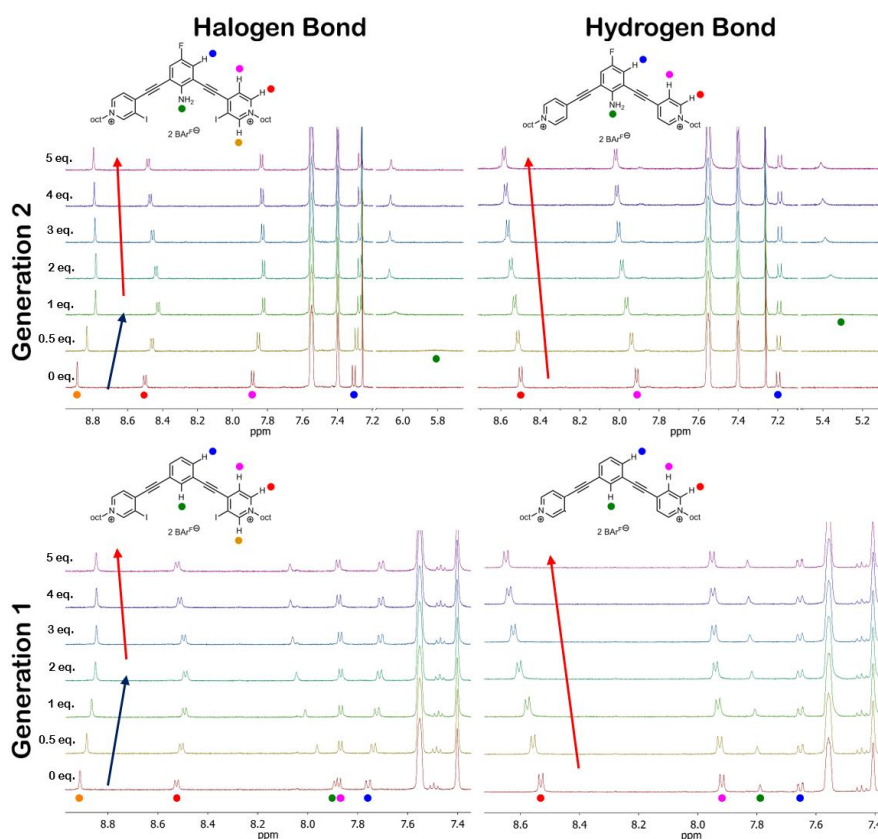


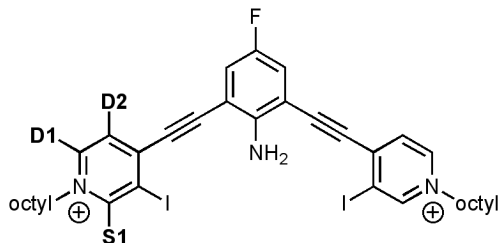
Figure S22. Stacked ^1H NMR of spectra of a titration of **G2XB**, **G2HB**, **G1XB** and **G1HB** with tetra-*n*-butylammonium iodide (60% CD_3NO_2 /40% CDCl_3 , 25°C, 500 MHz).

The K_{11} for each receptor is ascribed to the XB and HB interactions with each anion, while the K_{12} values are attributed to weak mono- and bidentate HB, weak σ -bonding and/or ion-pairing.² These binding modes are determined from the magnitude and direction of

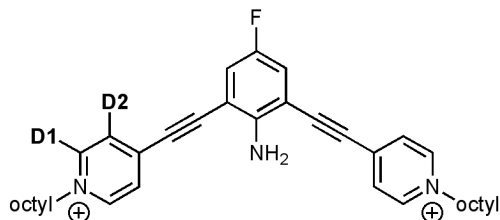
^1H shifts during the NMR titrations. Significant upfield shifting of pyridinium protons is indicative of XB in solution.³

NMR Titration Key. Signals followed in titration experiments are labeled with S1 (singlet 1), D1 (doublet 1), D2 (doublet 2), S2 (singlet 2), and D3 (doublet 3). Each proton signal was followed in each titration, however upon refinement of the data some signals were not used (lack of significant signal shift, causing a lot of error, or signals crossing) to fit the data as accurately as possible.

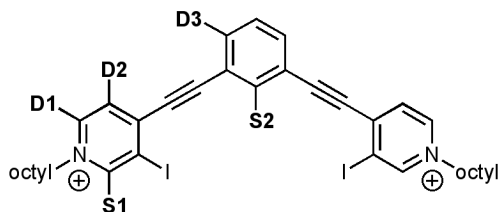
G2XB²⁺



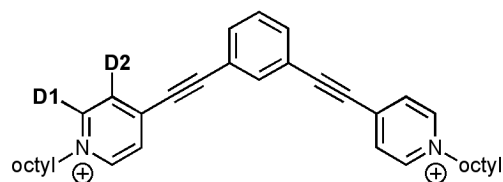
G2HB²⁺



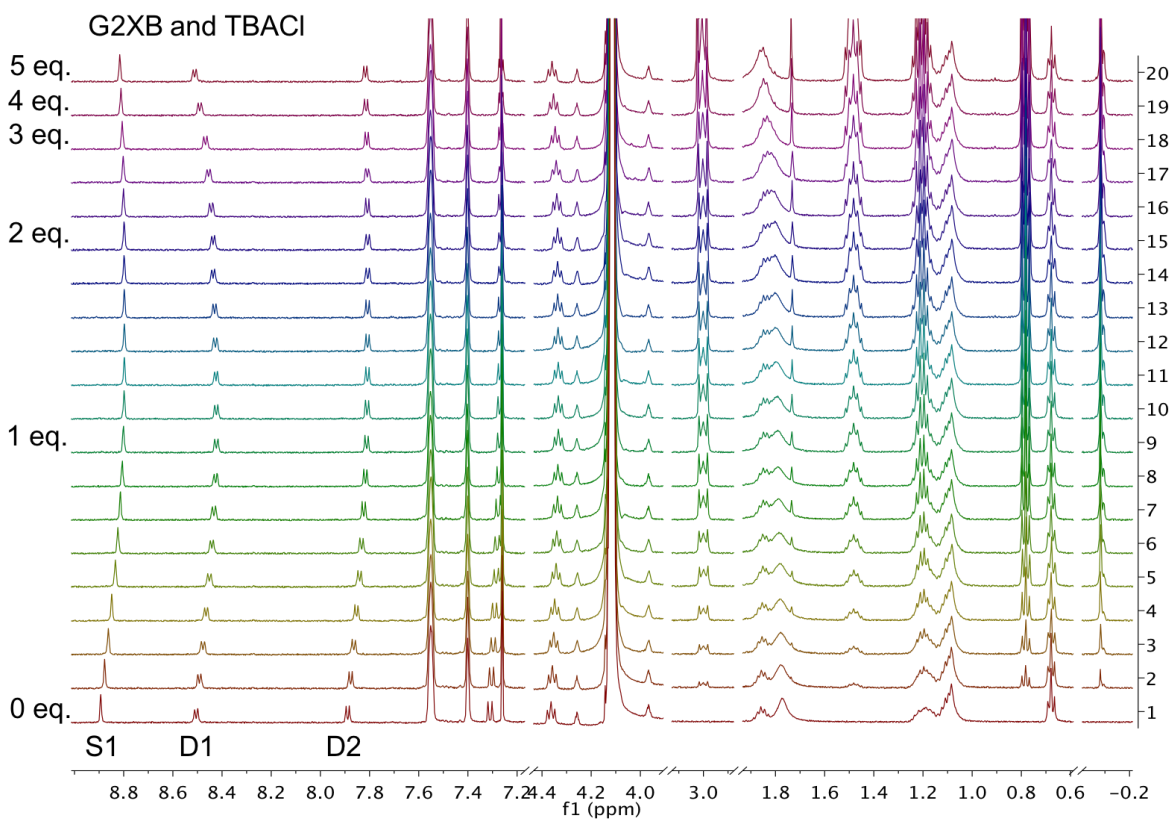
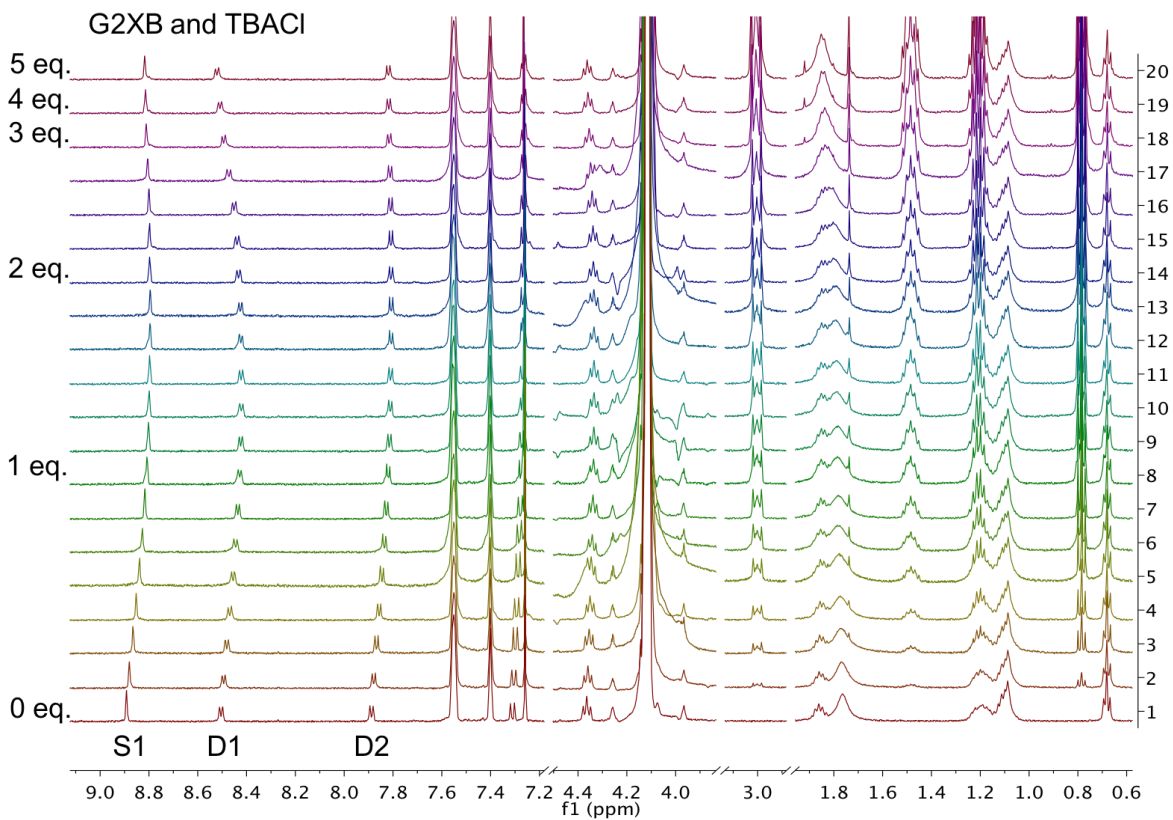
G1XB²⁺

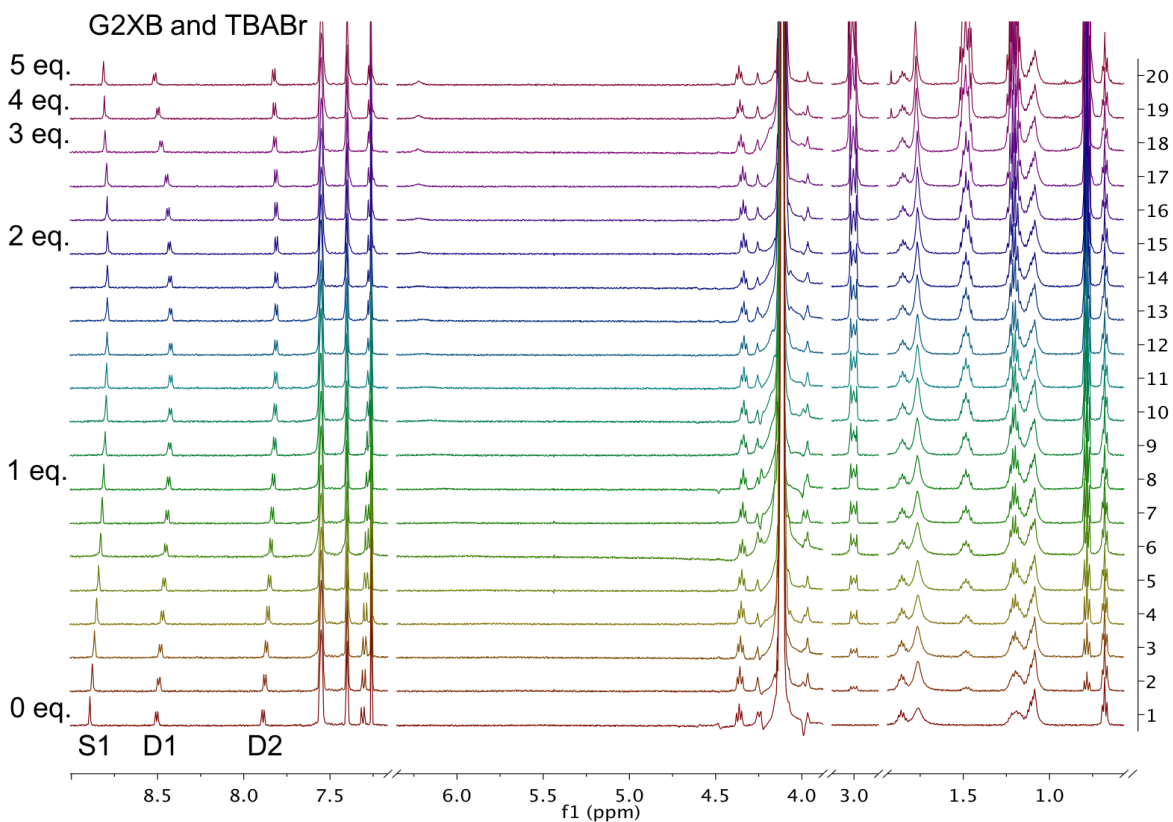
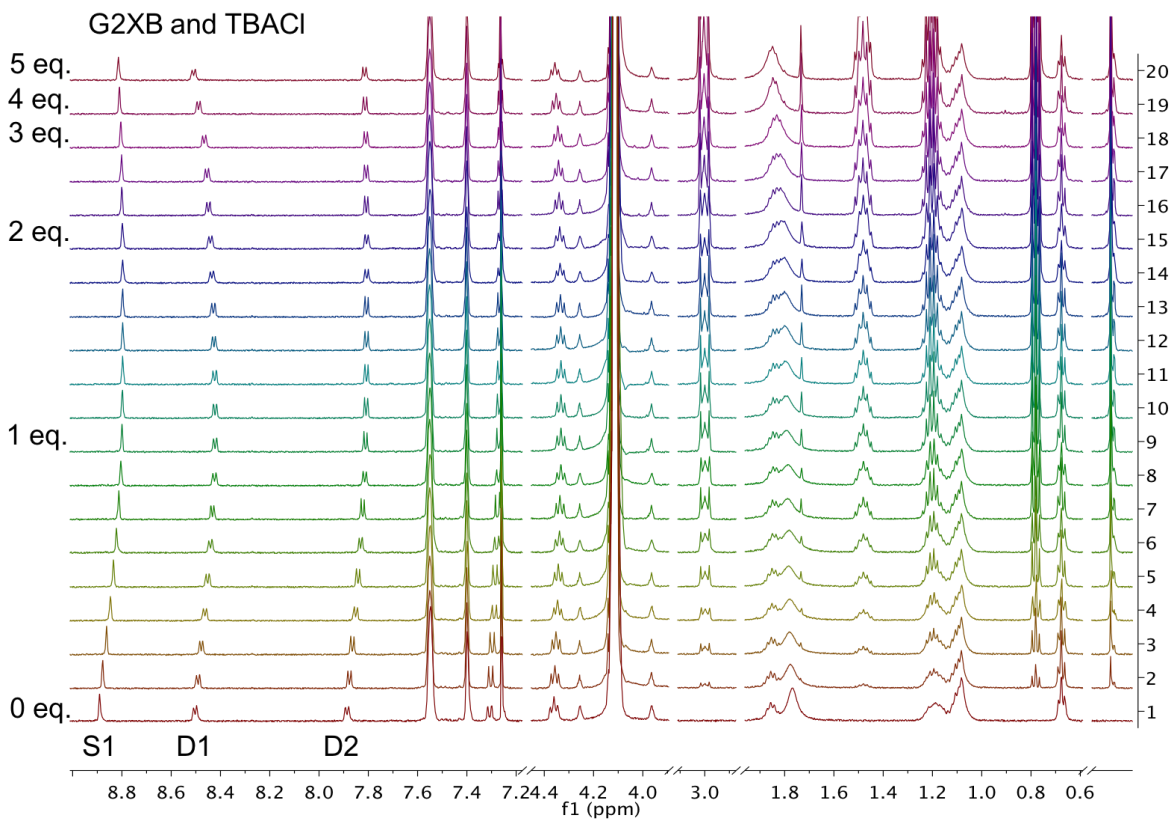


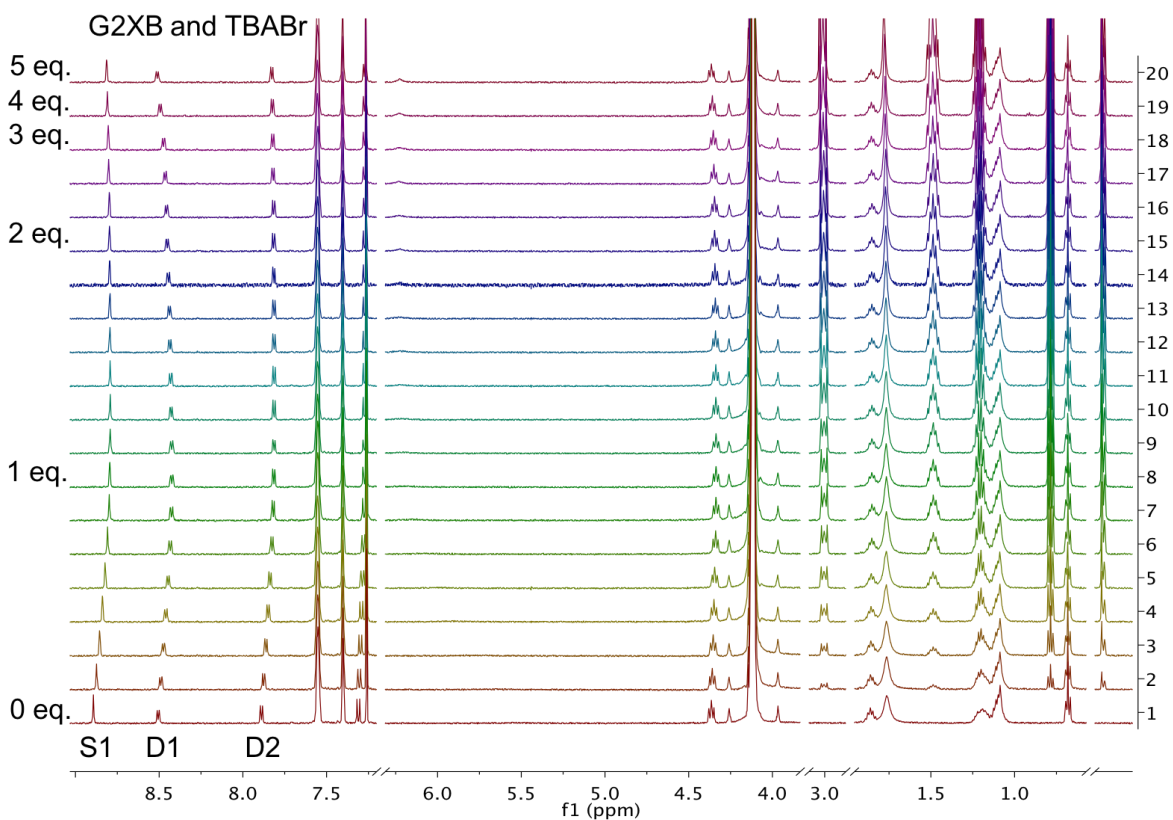
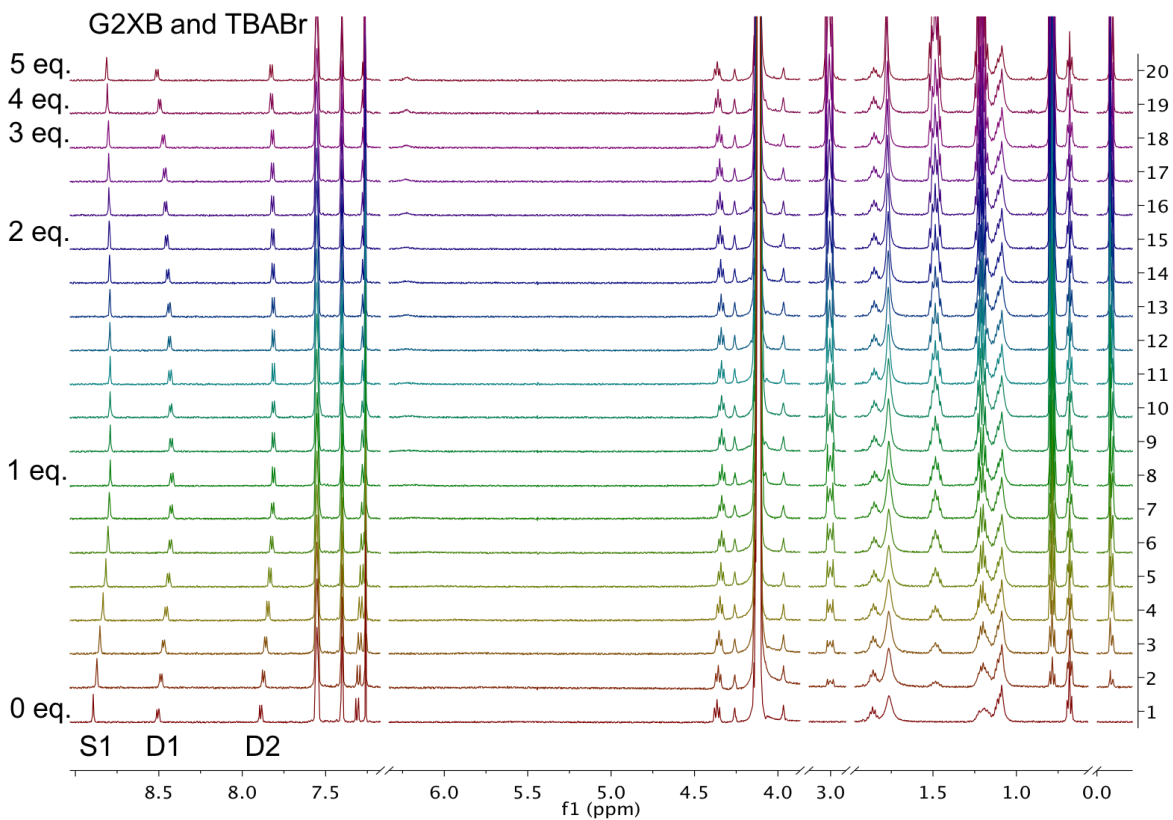
G1HB²⁺

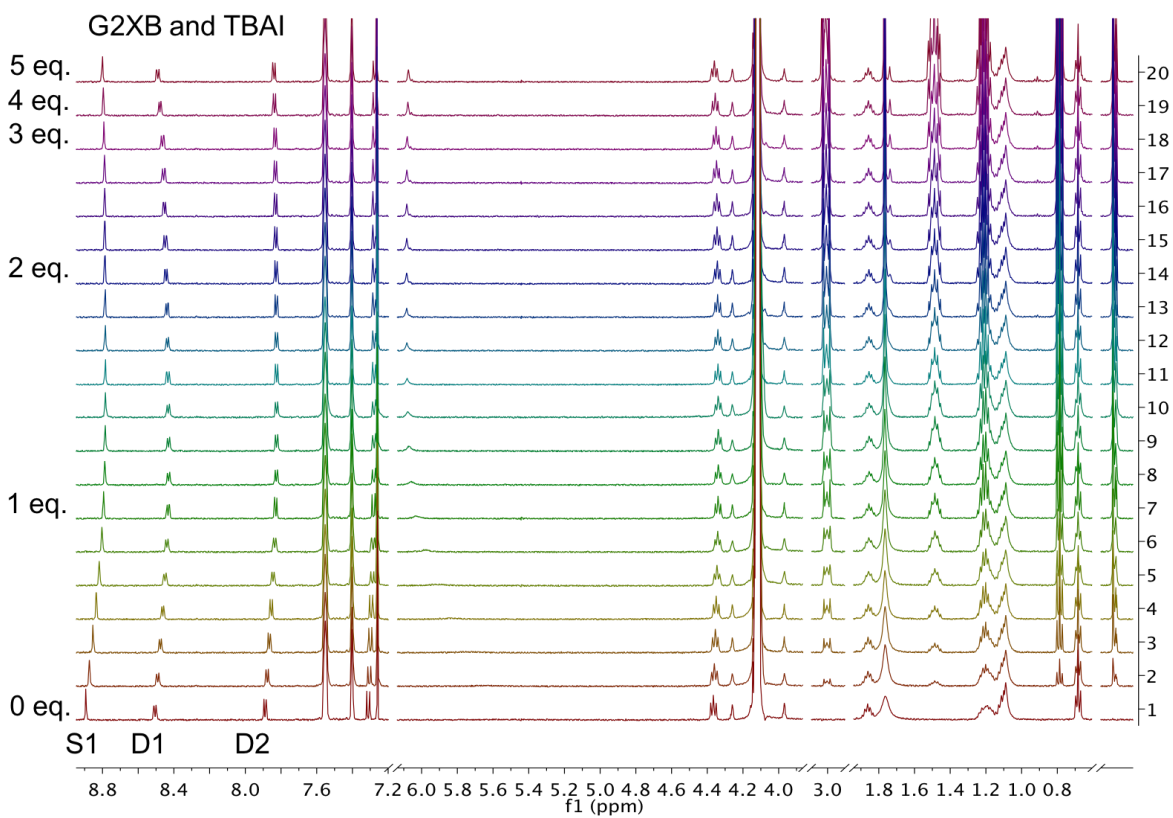
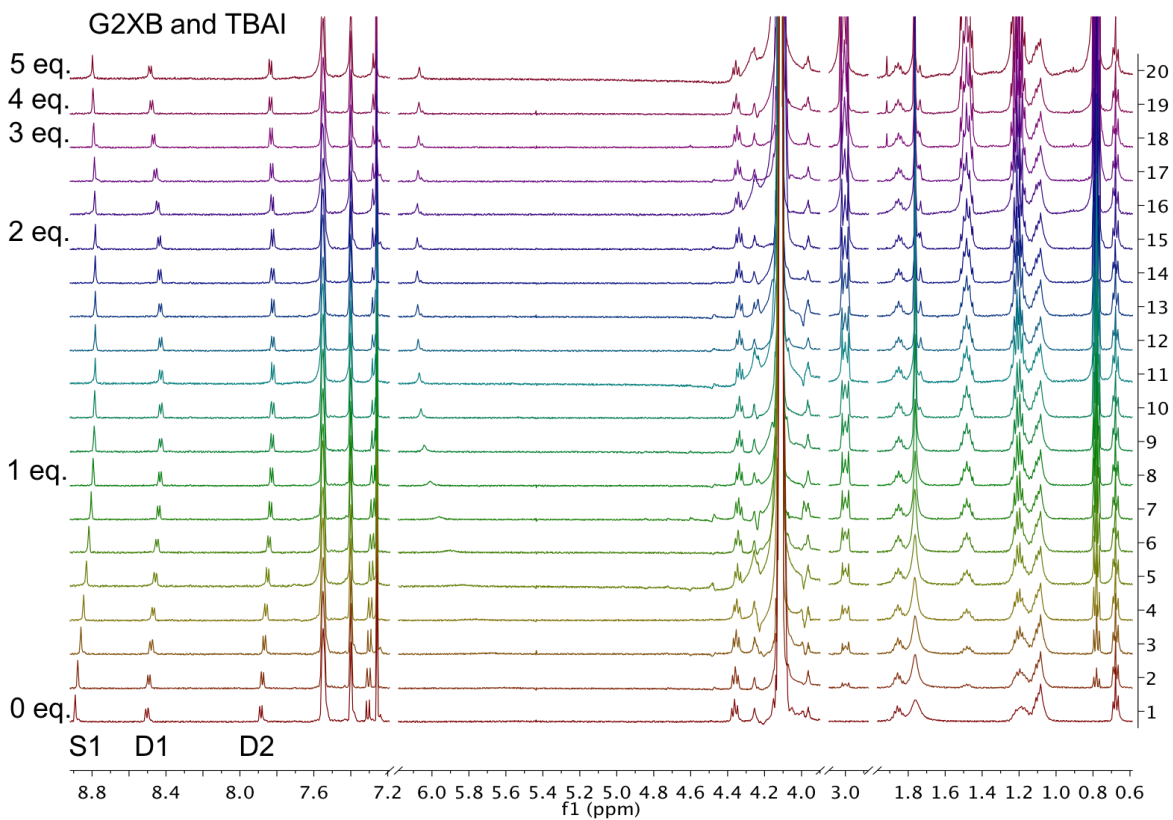


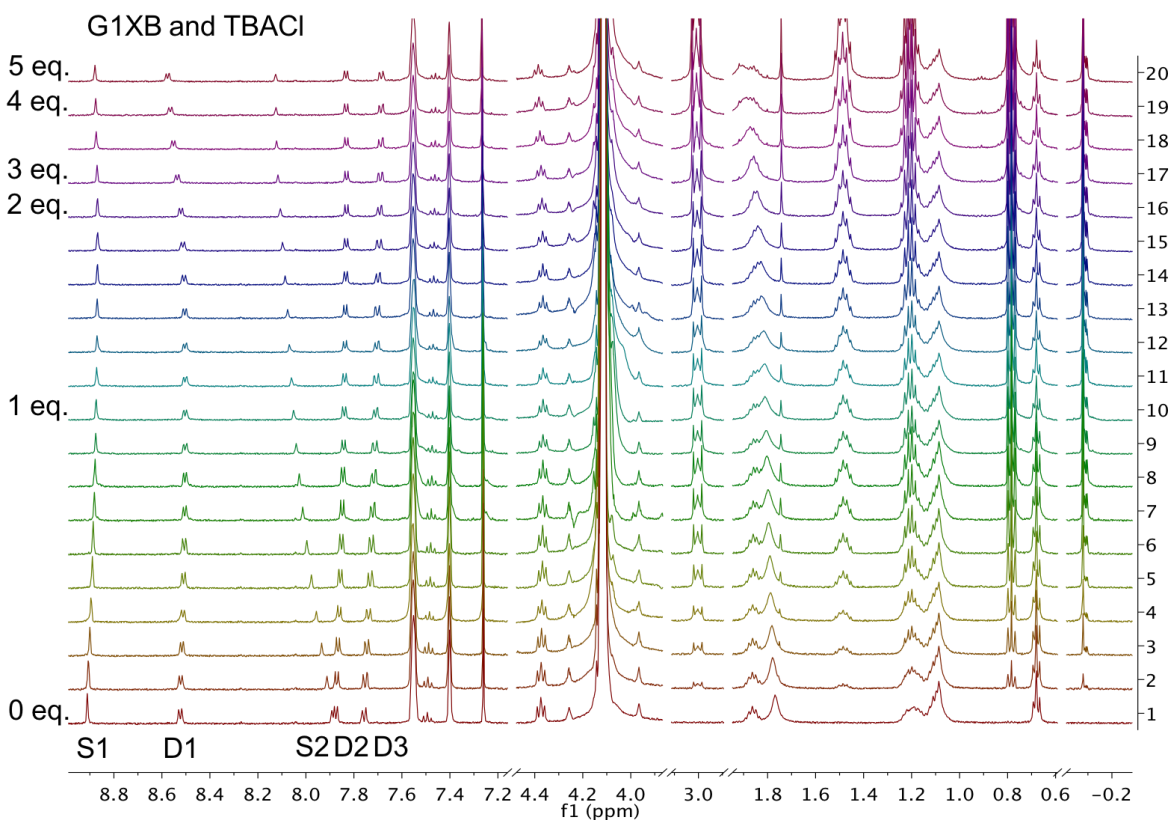
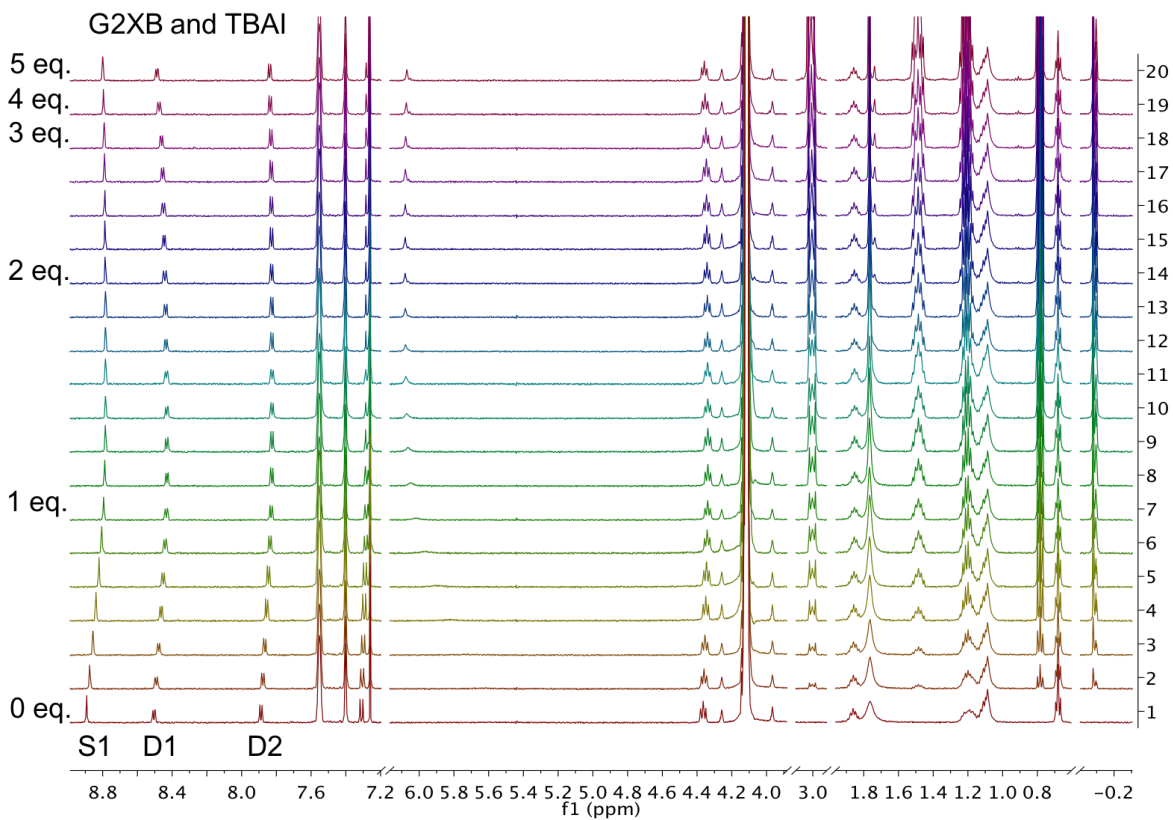
Stacked NMR Titrations. NMR stacks are given in triplicate. Peaks potentially followed for refinement are labeled below the stack as S1, D2, etc. Guest equivalents are displayed on the left of the stacked spectra.

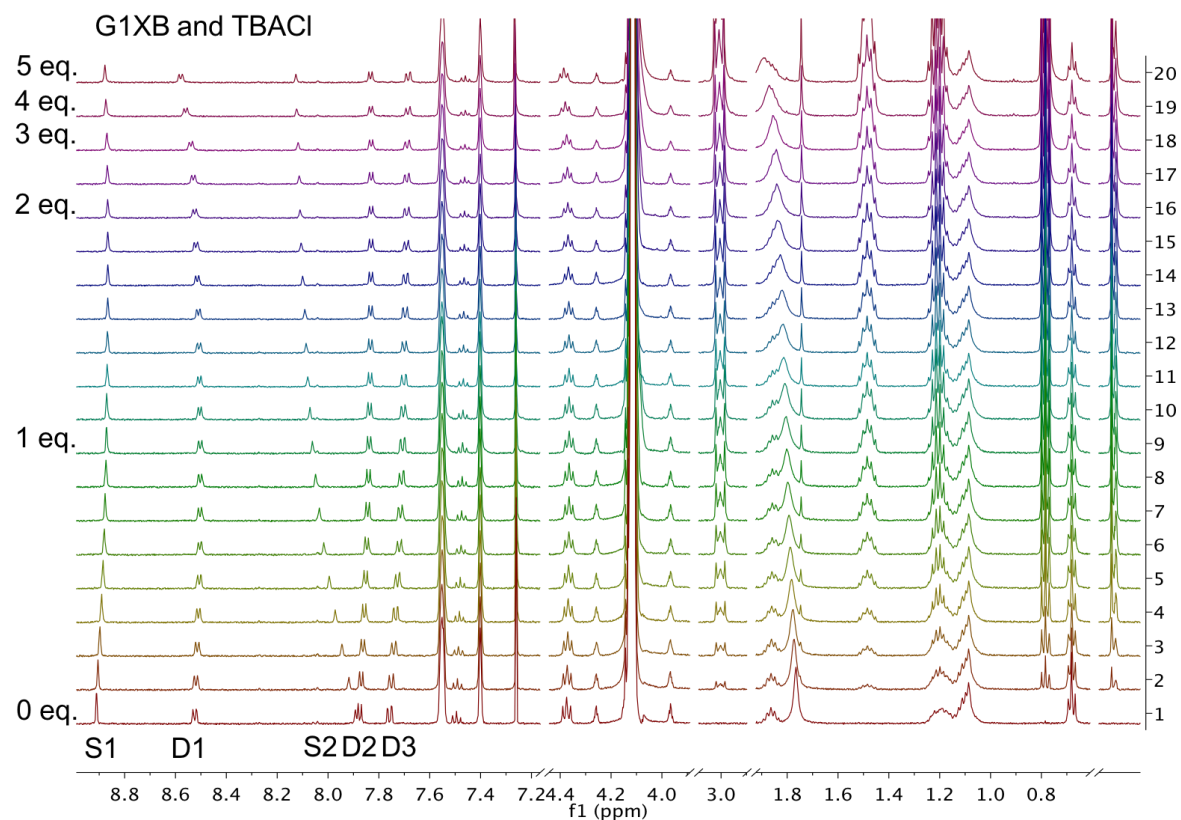
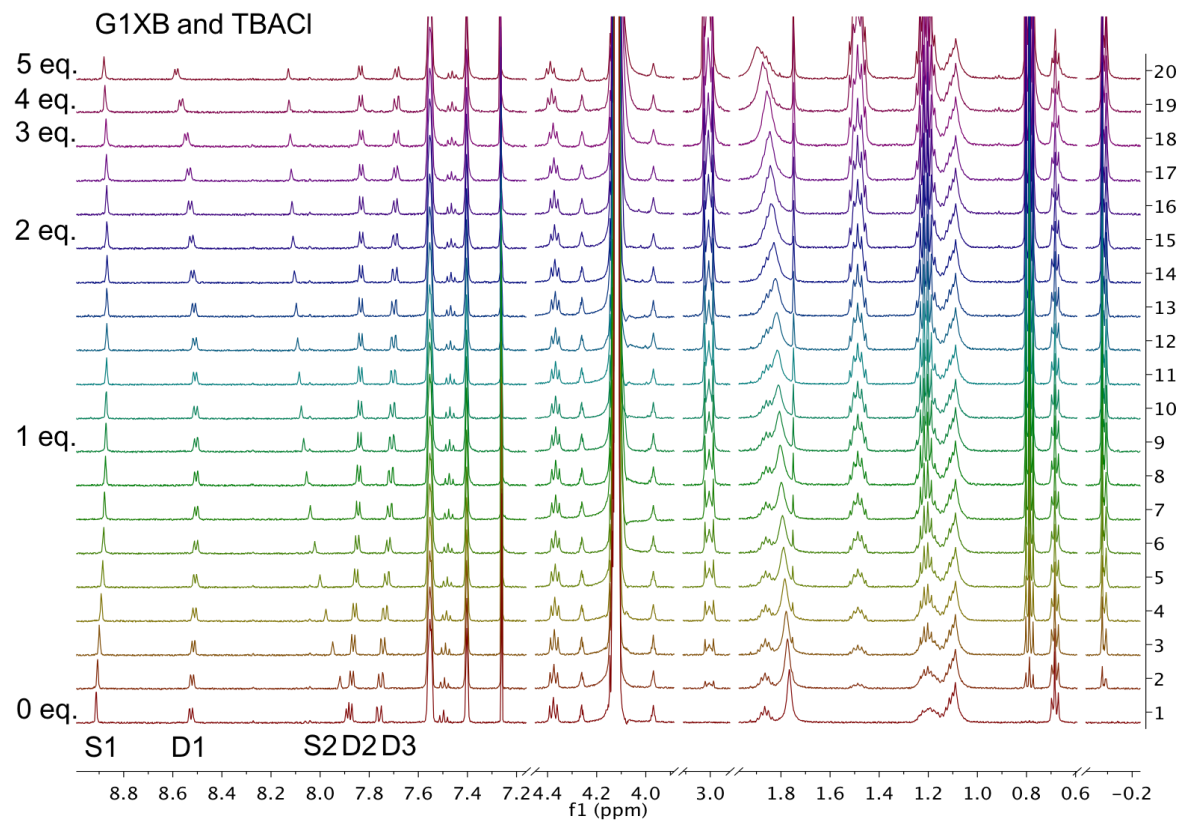


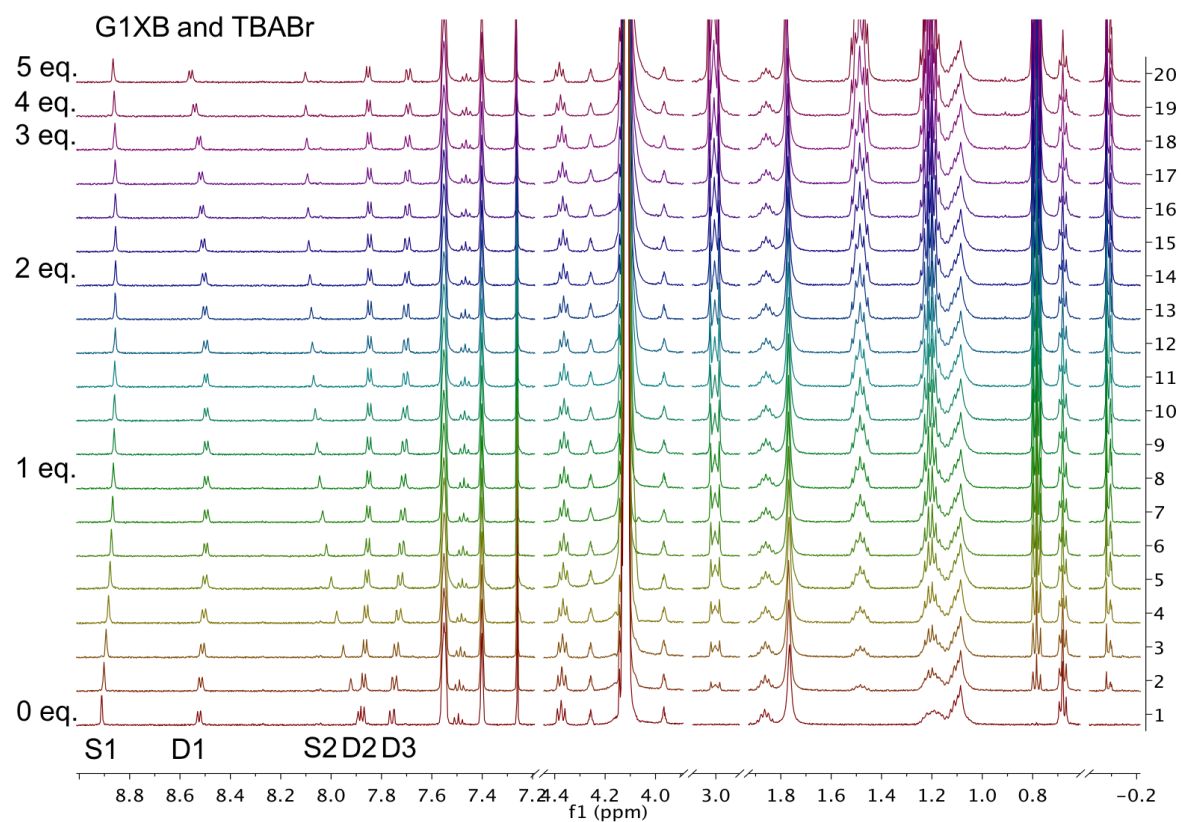
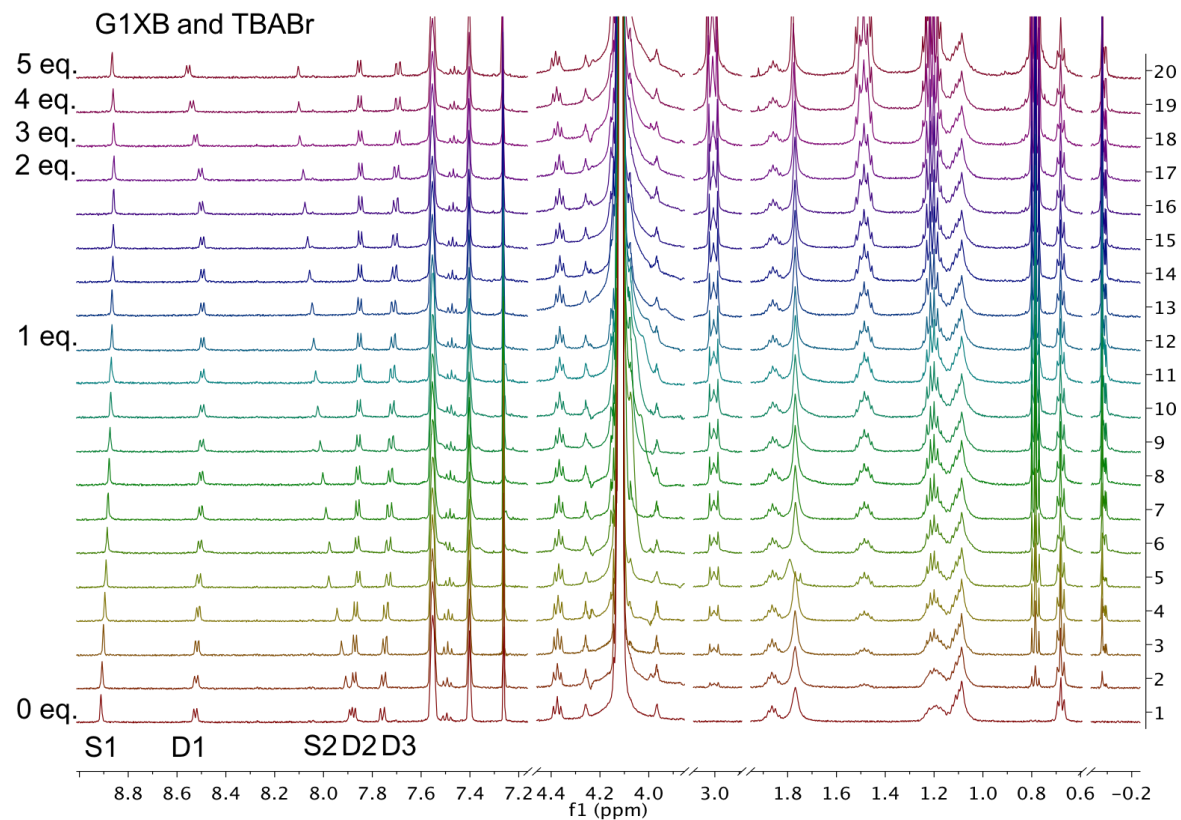


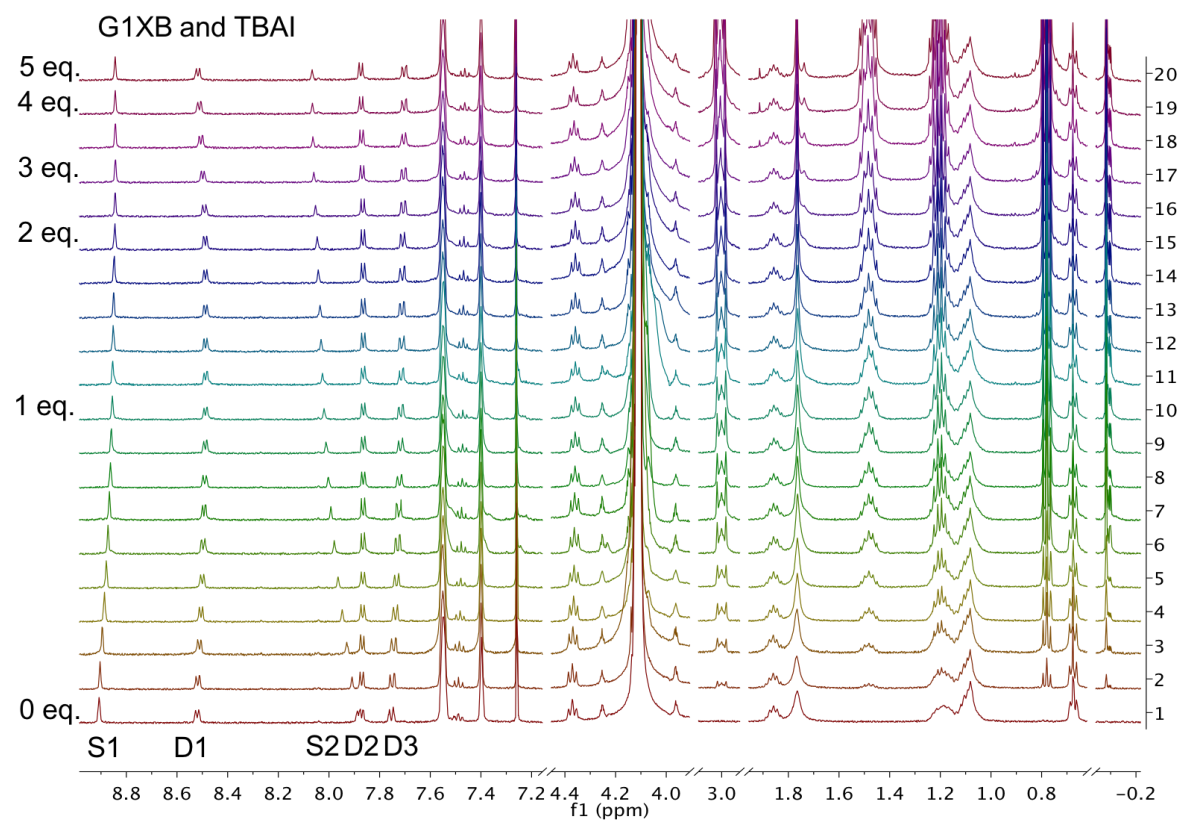
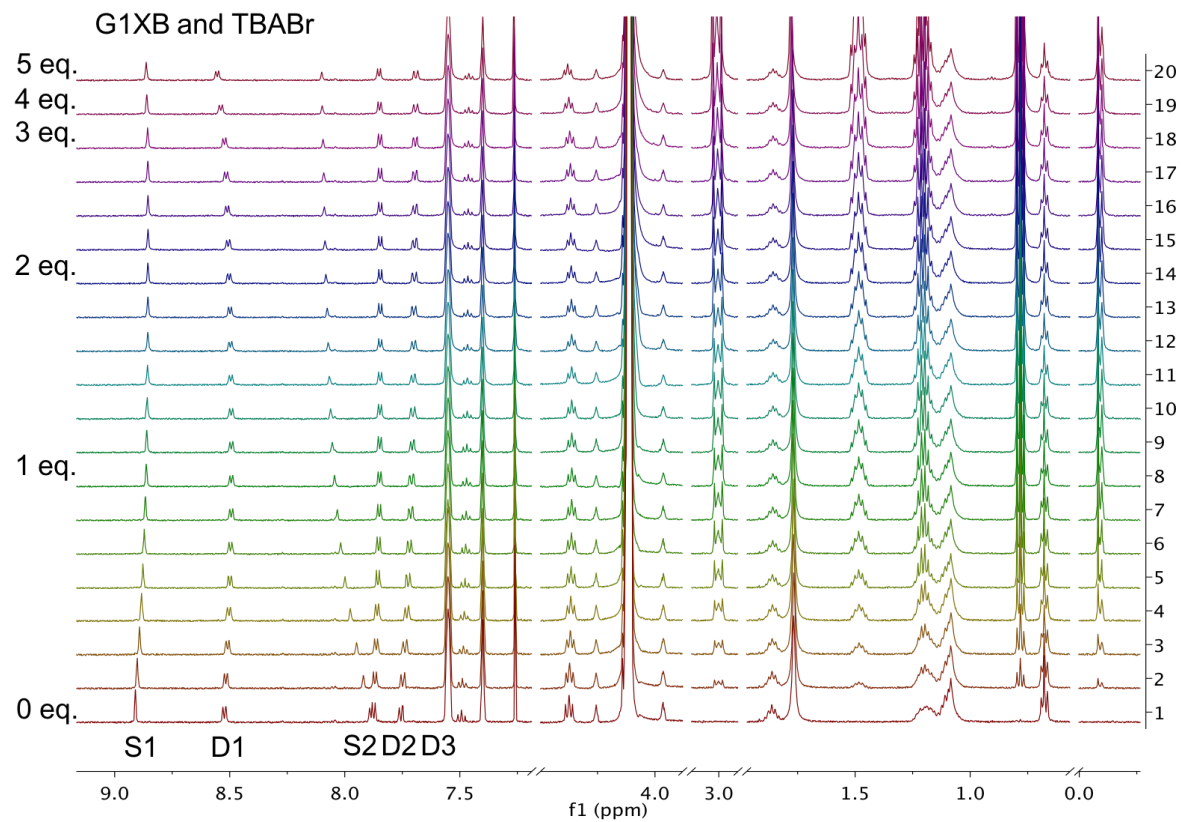


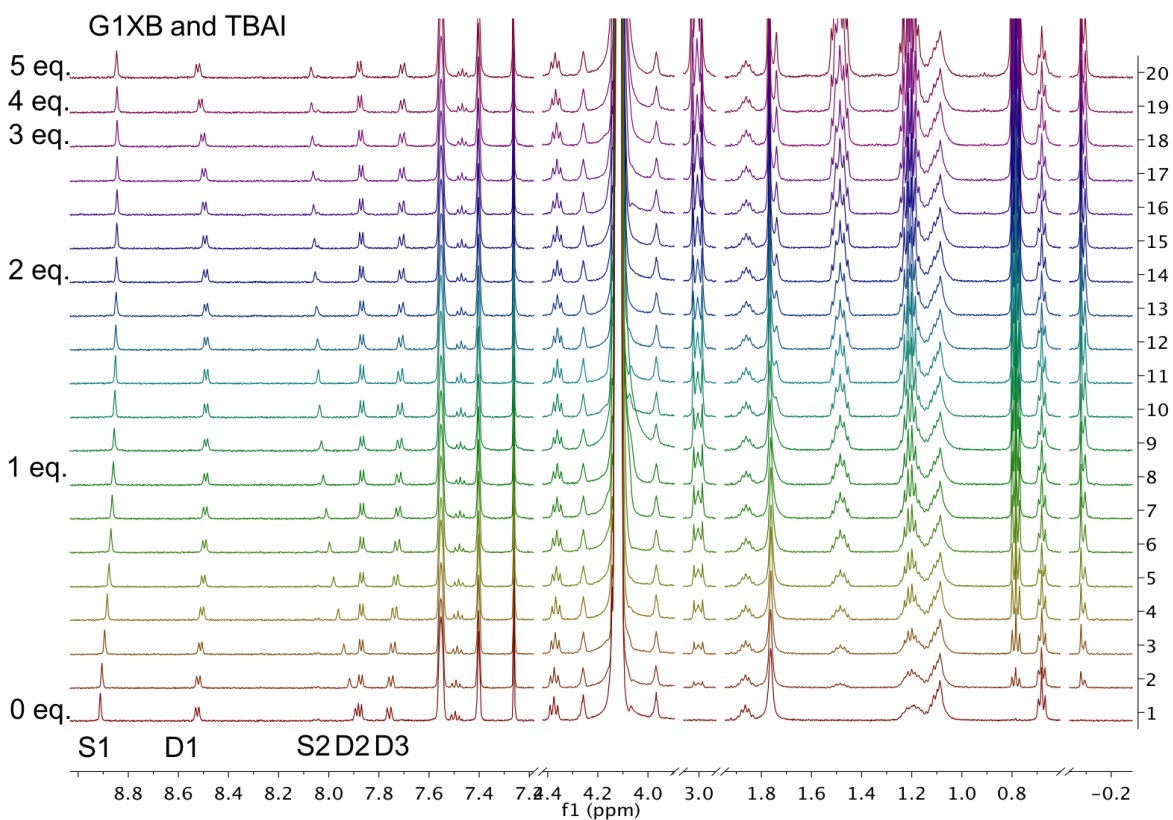
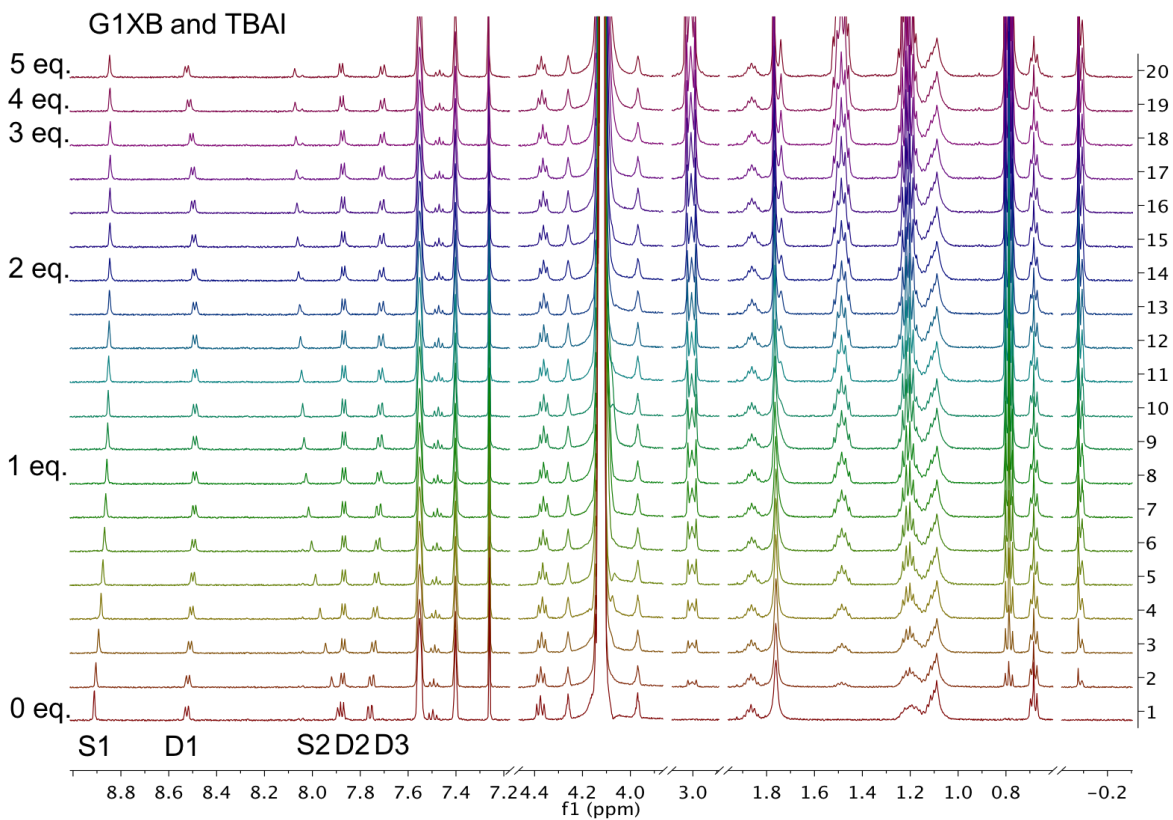


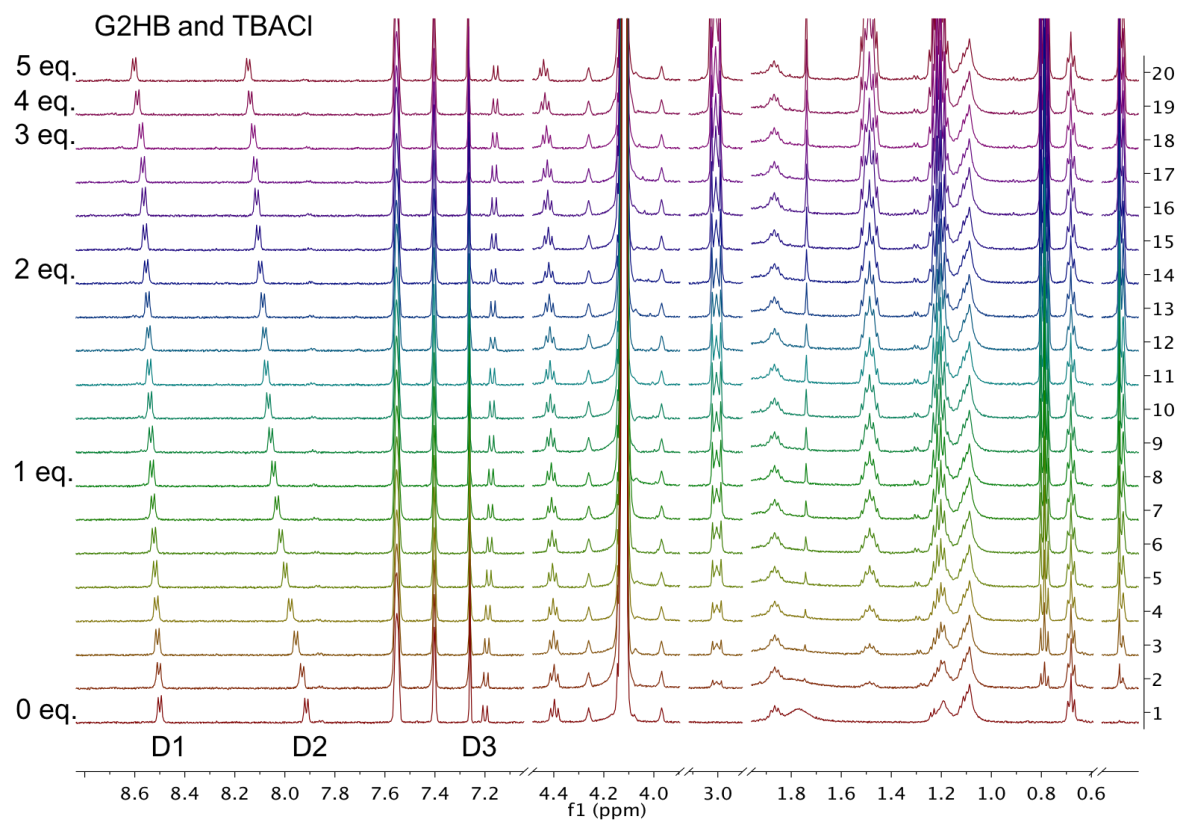
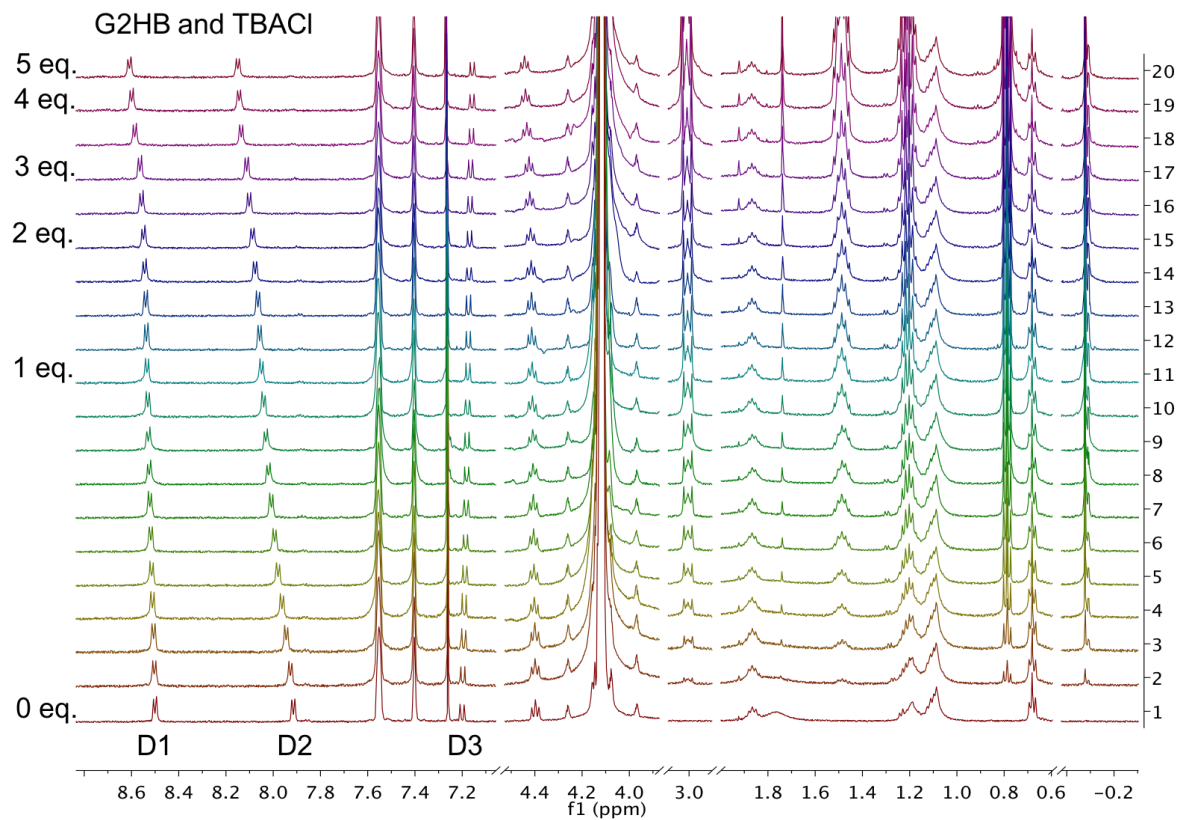


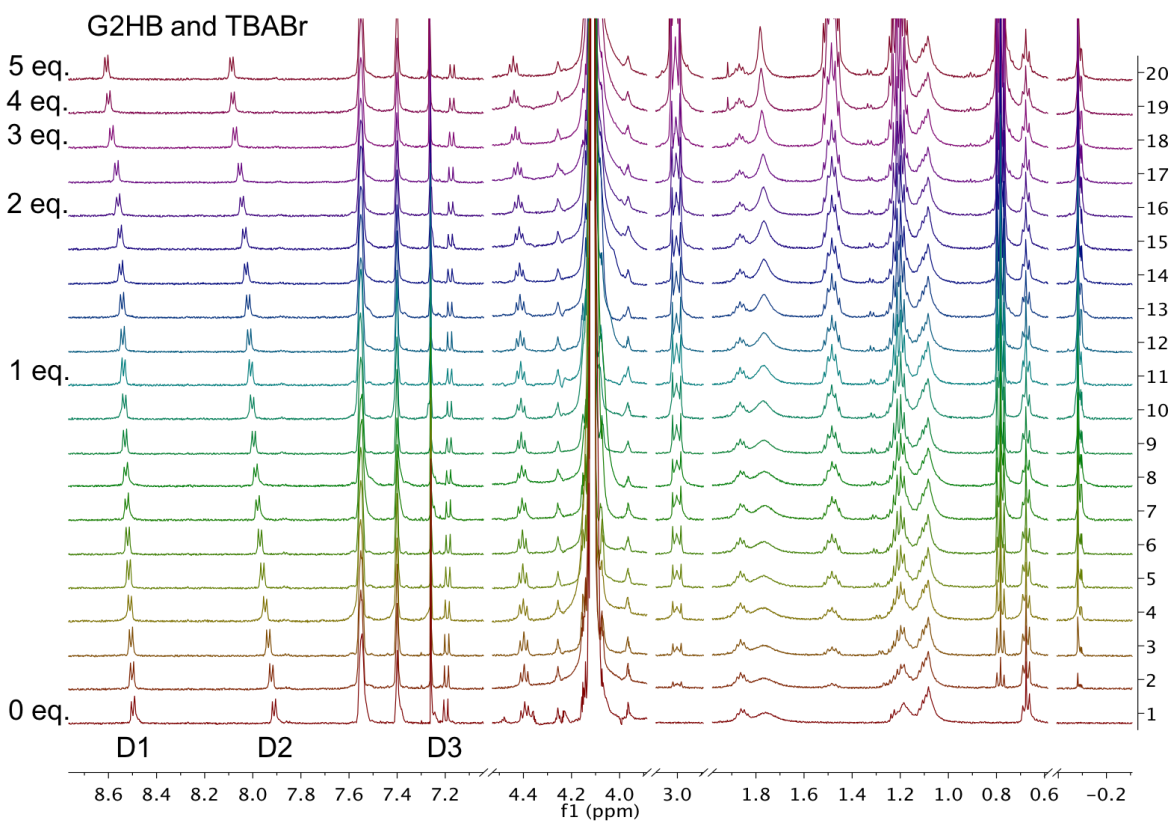
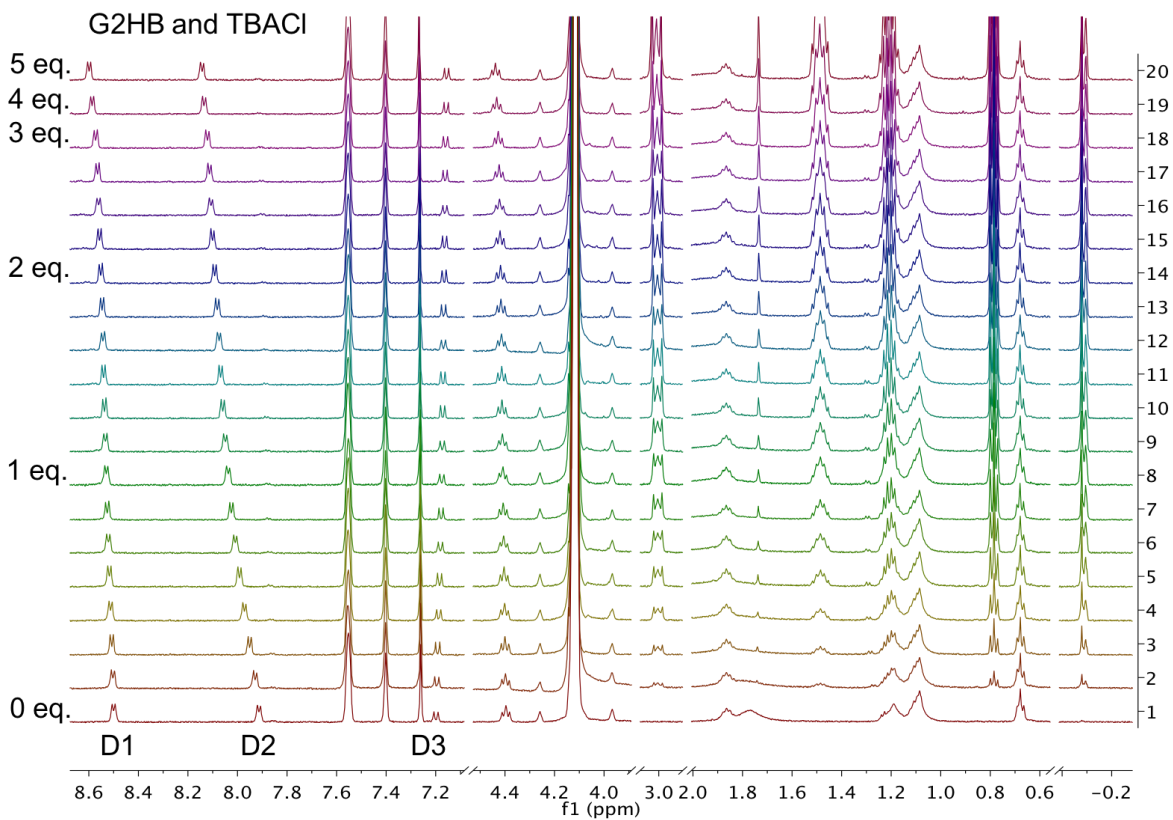


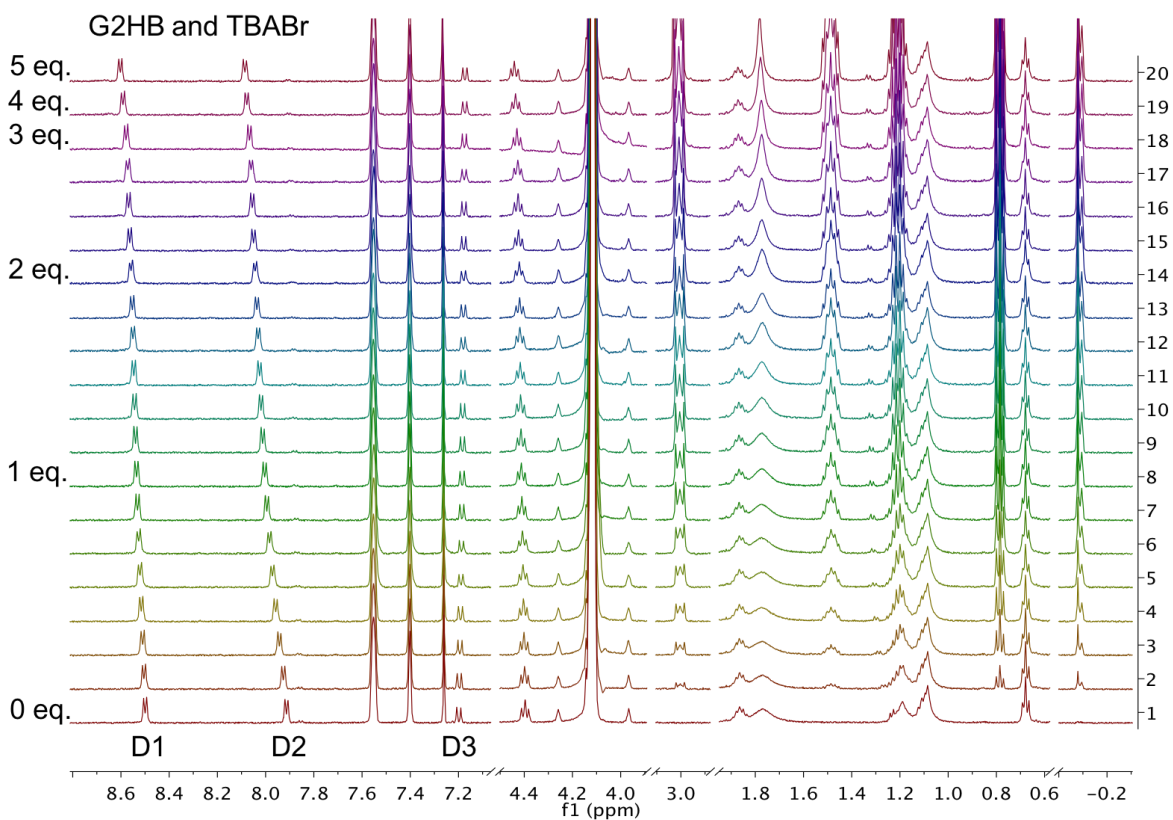
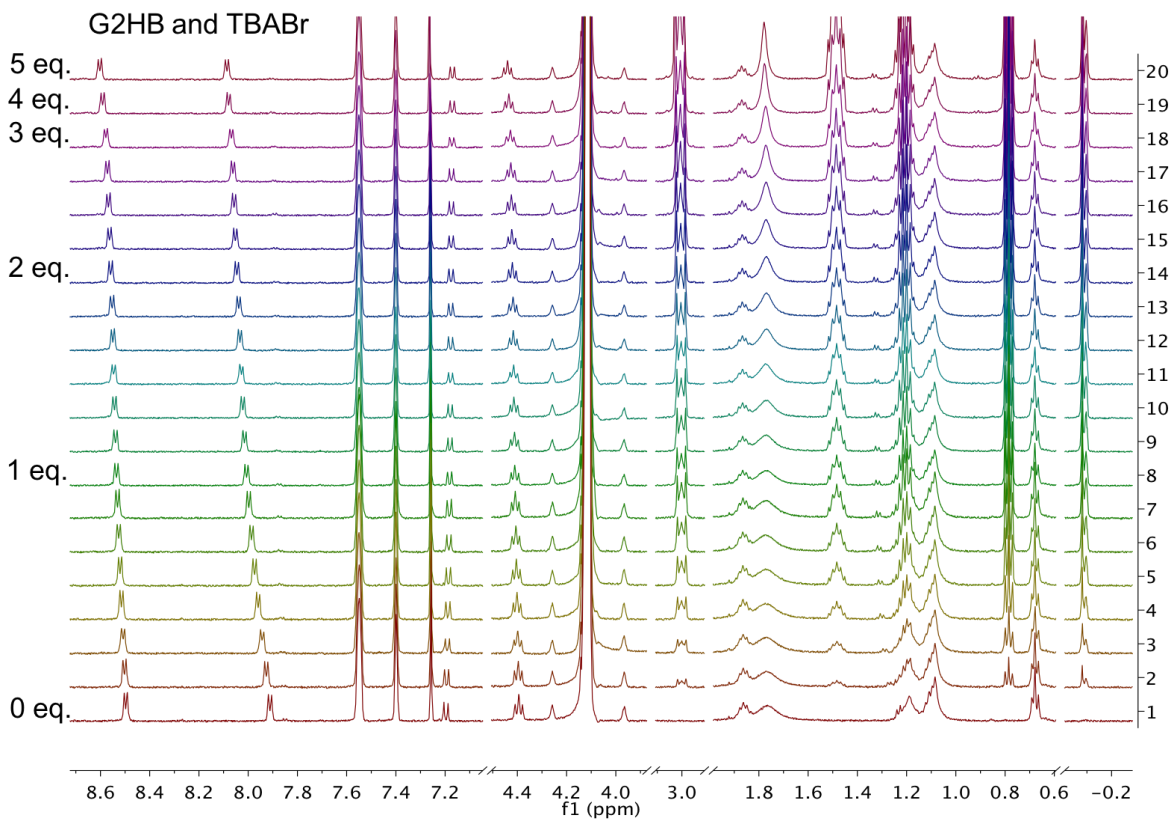


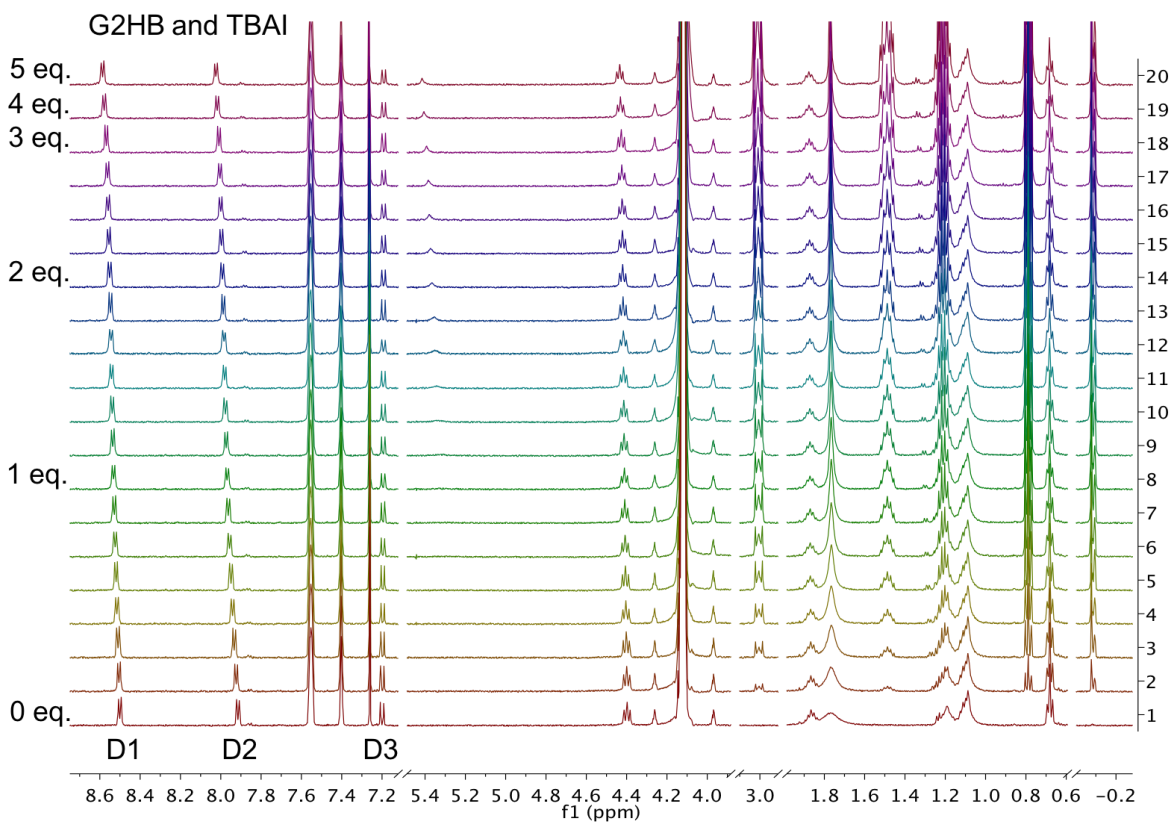
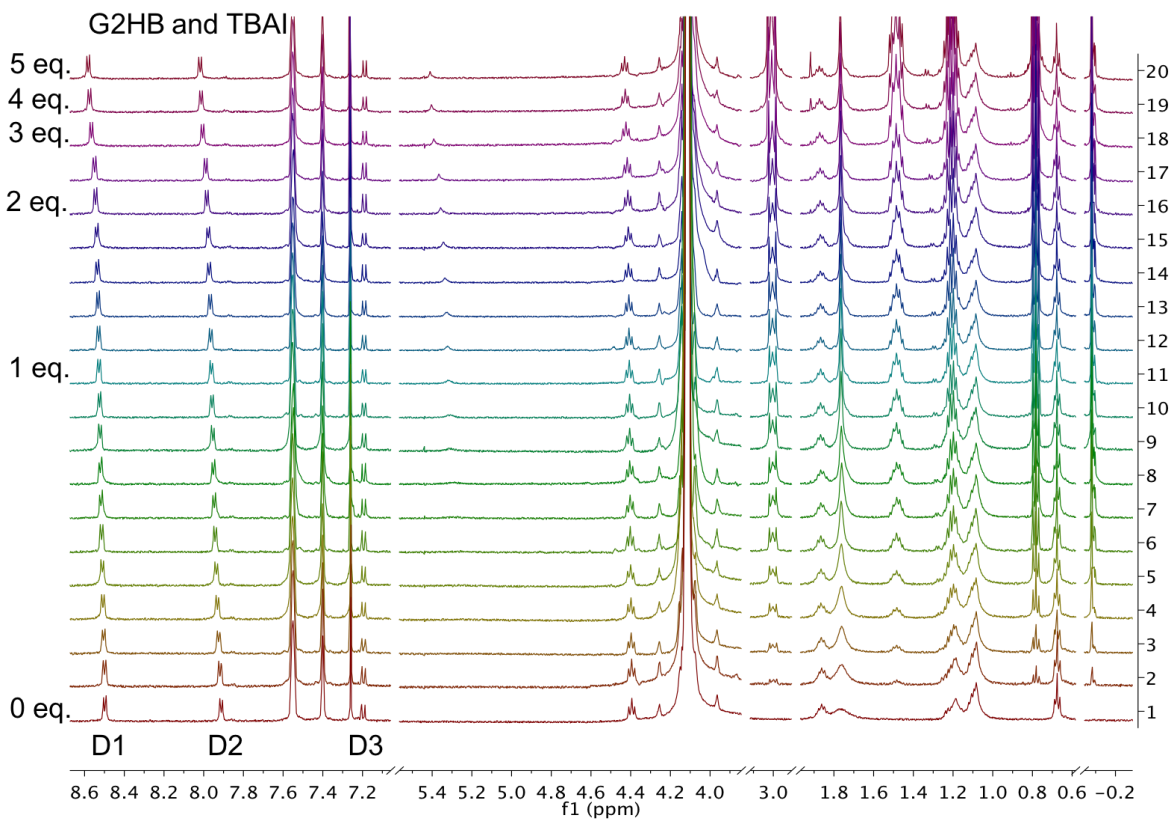


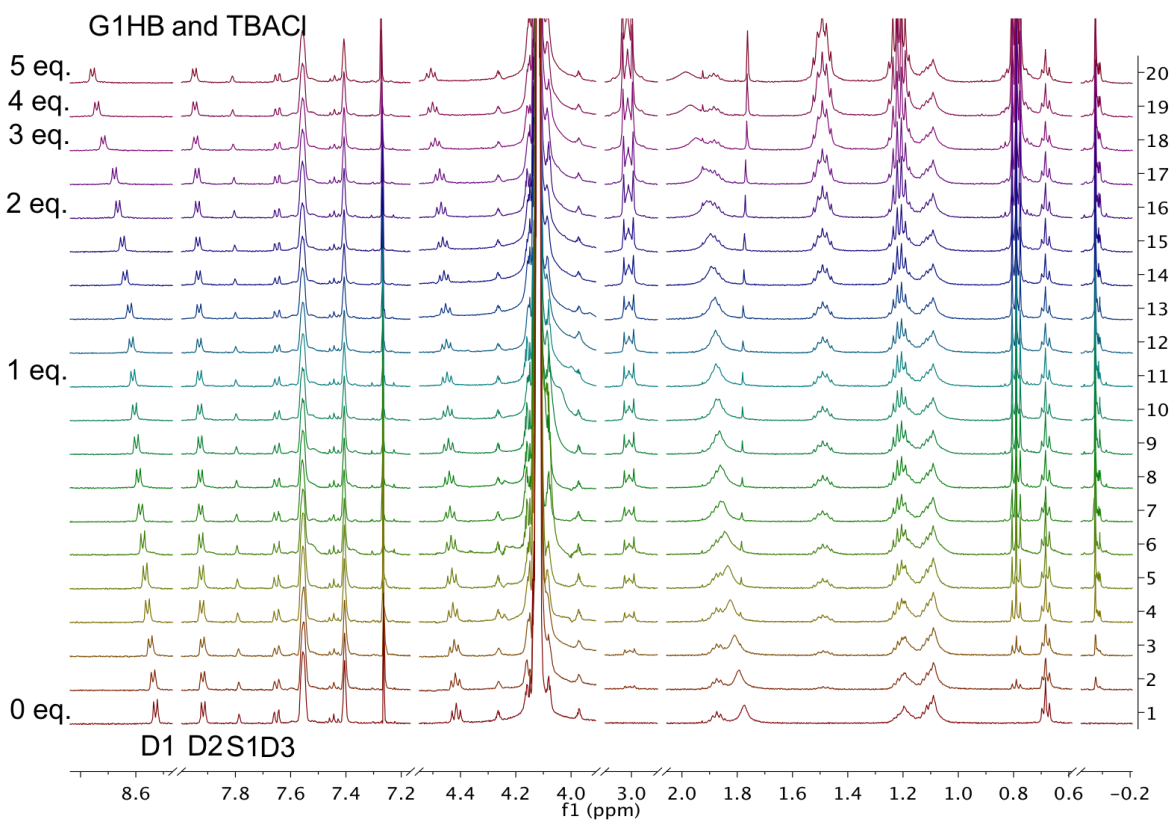
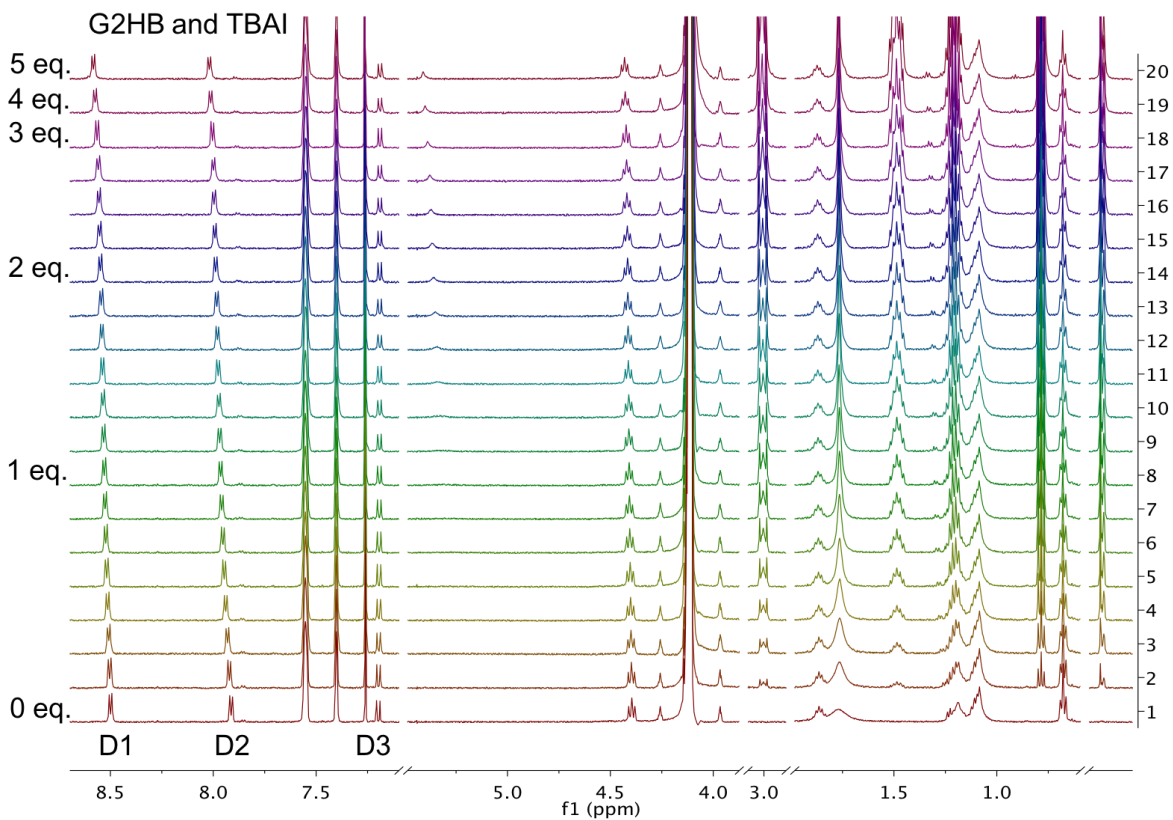


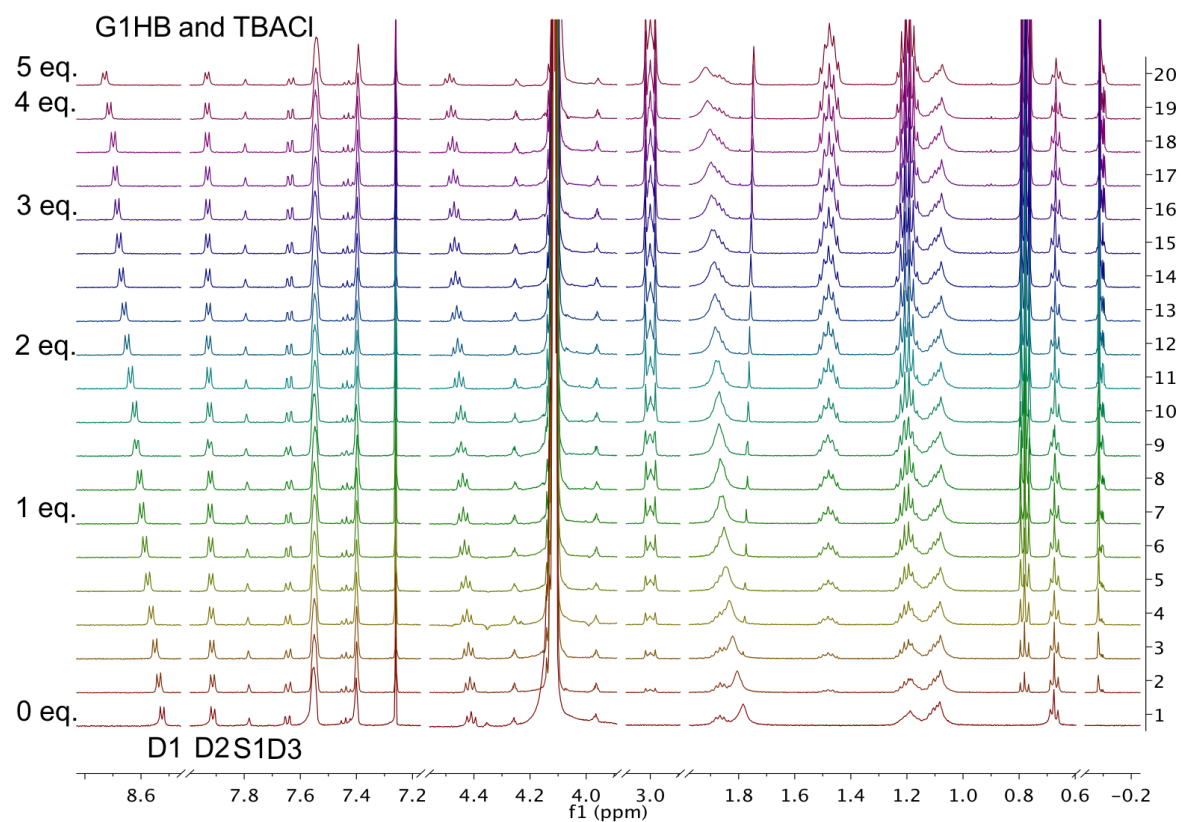
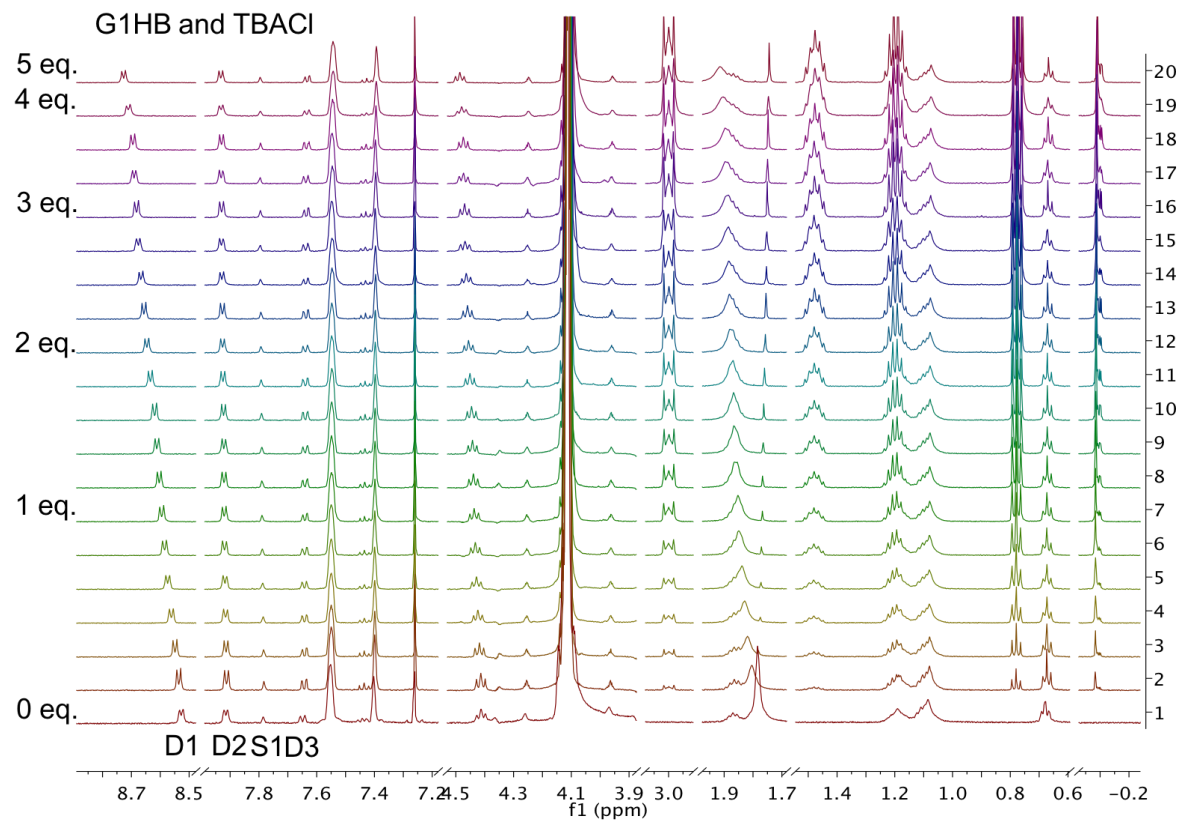


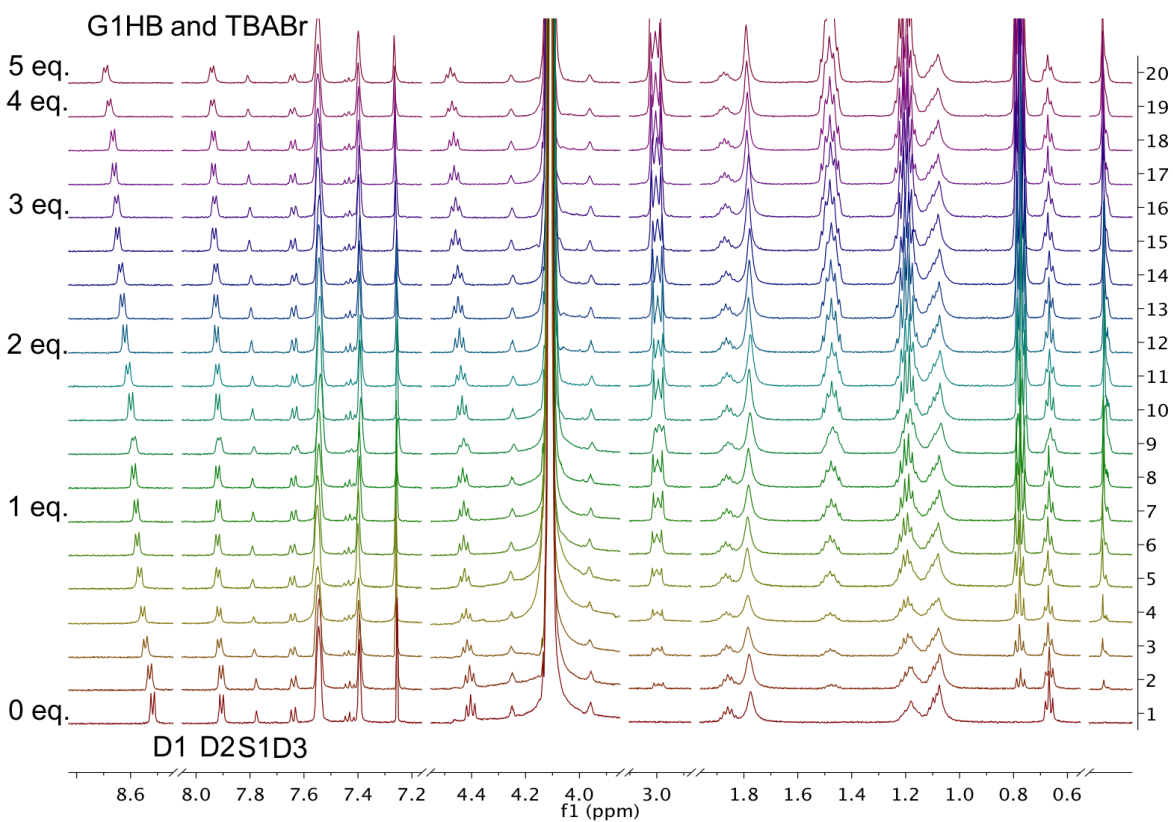
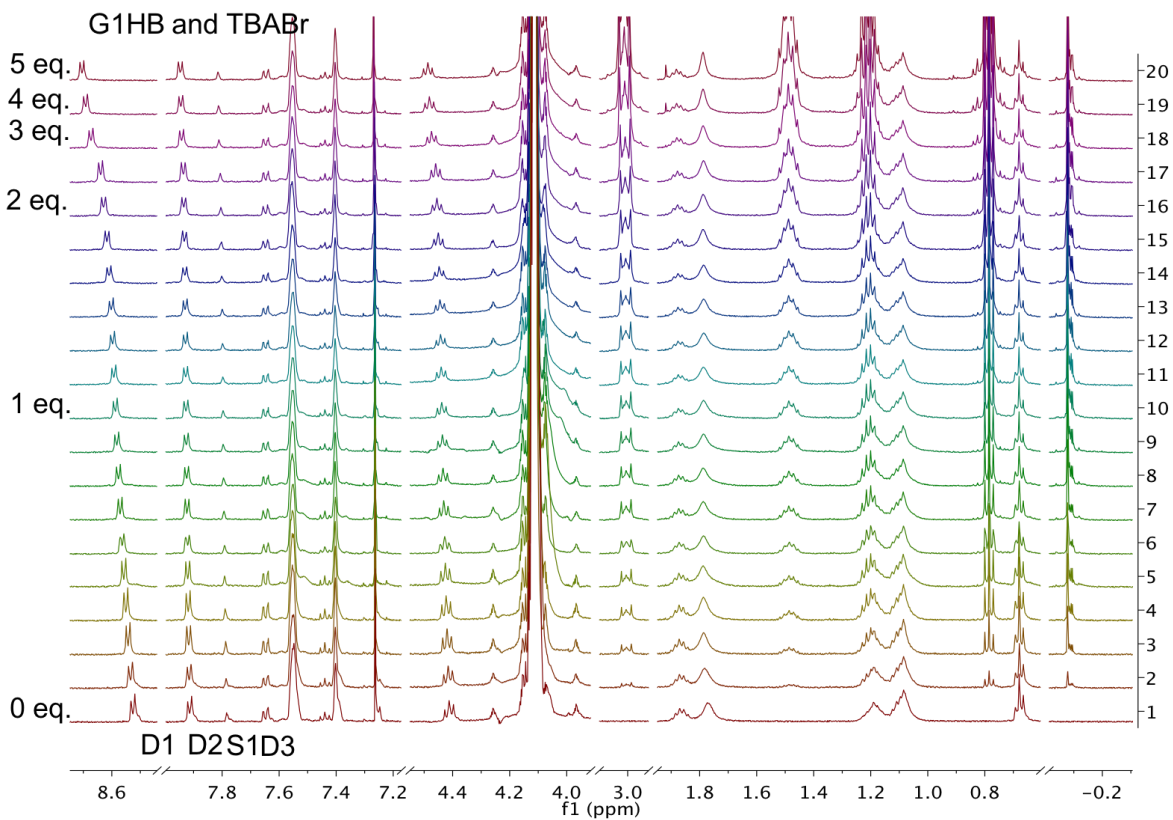


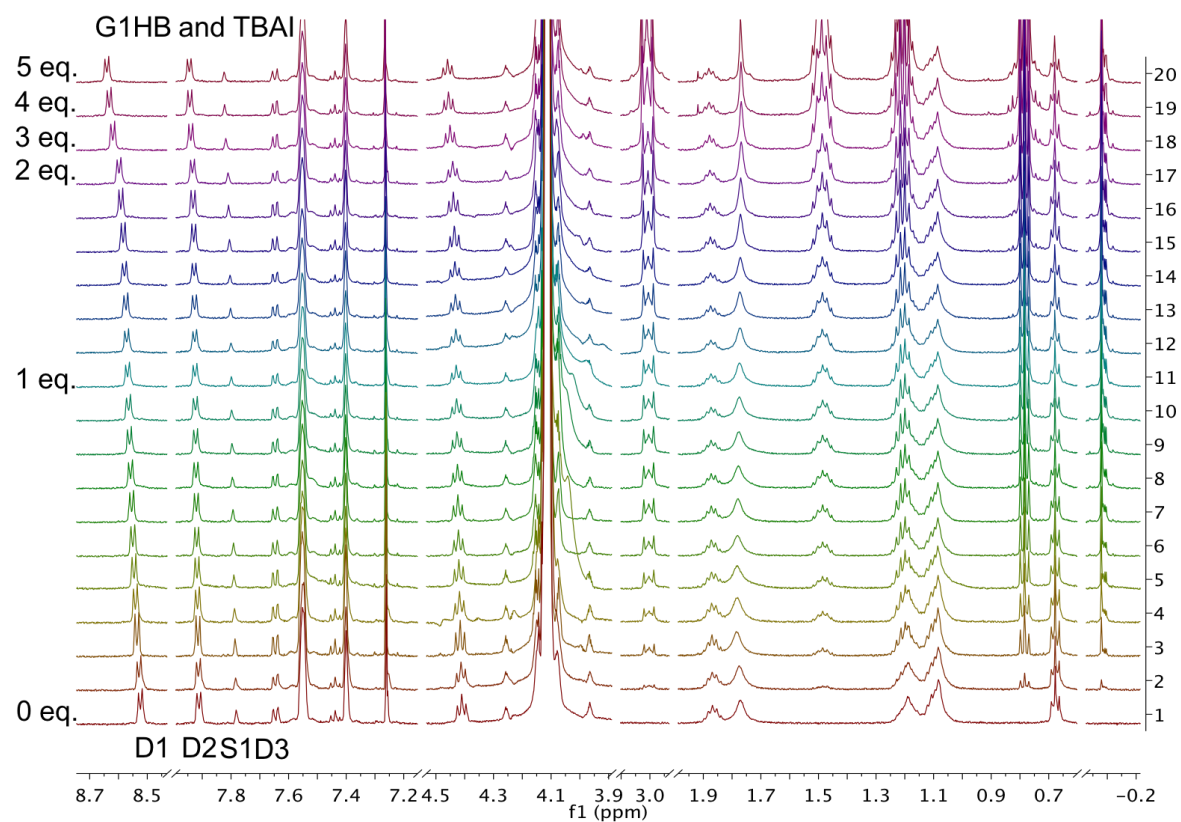
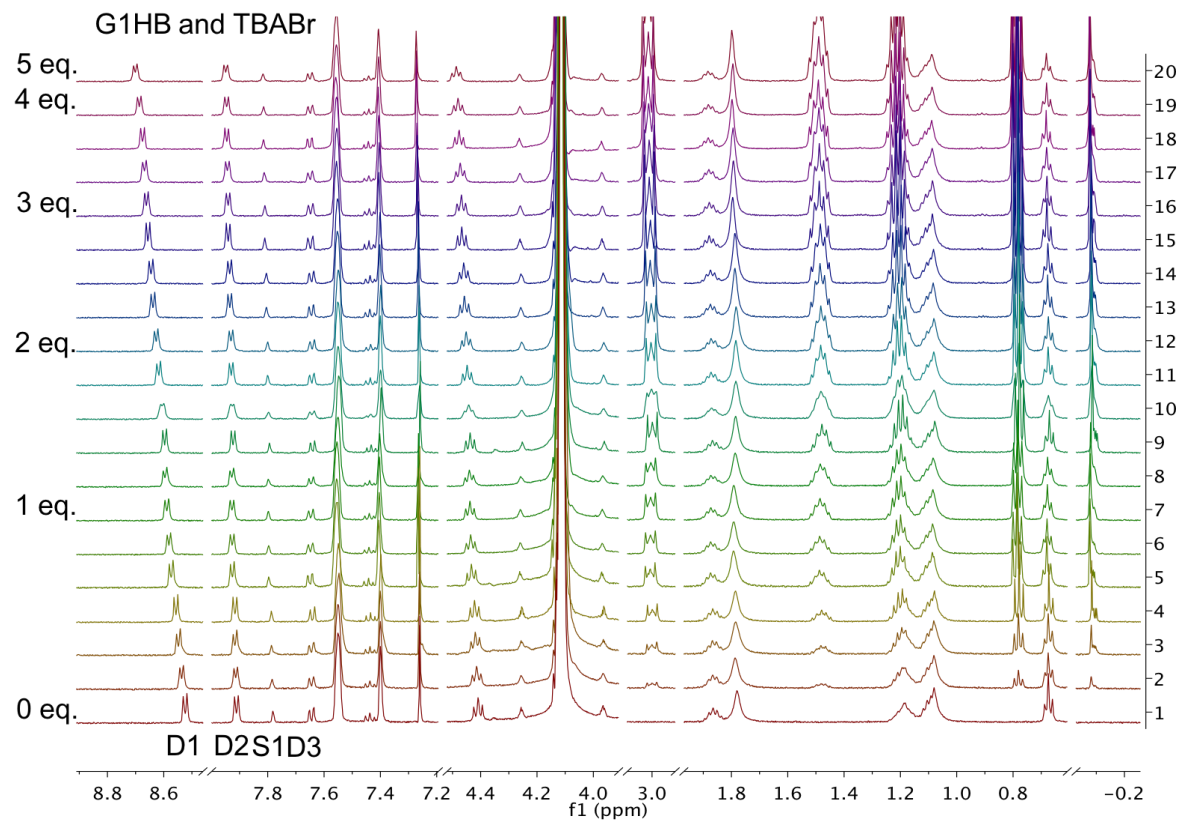


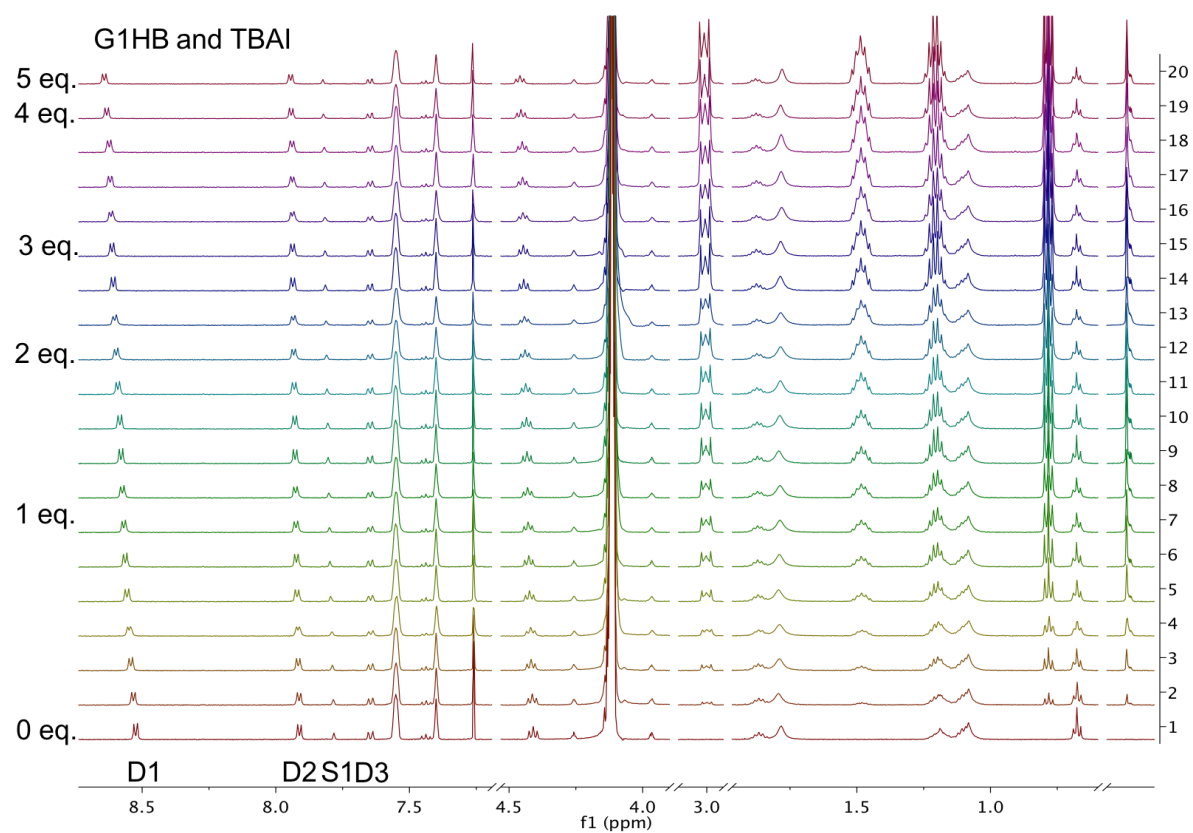
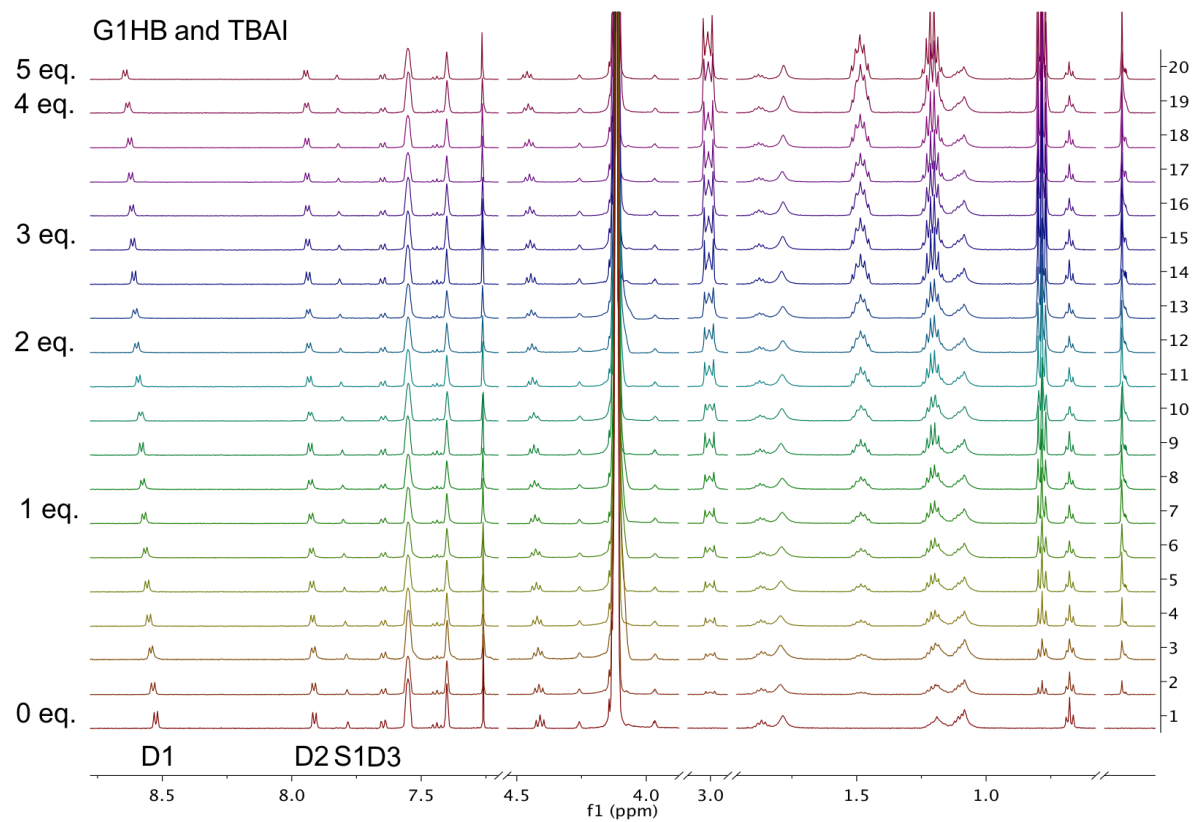












Hyp NMR Output Files and Graphs

G2XB and TBA⁺Cl⁻ (Experiment 1)

Species	Log beta	G	H	std. dev.
1	4.2711	1	1	0.0836
2	5.8942	2	1	0.1194

Converged in 1 iterations with sigma = 0.159039

Species concentrations/mol dm⁻³

Point	pH	T(TBACl)	T(G2XB)	F(TBACl)	F(G2XB)	species 1	species 2
1	-	0.00E+00	1.56E-03	3.45E-91	1.56E-03	1.01E-89	1.46E-178
2	-	2.25E-04	1.56E-03	8.61E-06	1.35E-03	2.17E-04	7.83E-08
3	-	4.46E-04	1.56E-03	2.00E-05	1.14E-03	4.26E-04	3.58E-07
4	-	6.63E-04	1.56E-03	3.57E-05	9.38E-04	6.25E-04	9.38E-07
5	-	8.76E-04	1.56E-03	5.82E-05	7.49E-04	8.13E-04	1.99E-06
6	-	1.08E-03	1.56E-03	9.16E-05	5.76E-04	9.85E-04	3.79E-06
7	-	1.29E-03	1.56E-03	1.43E-04	4.25E-04	1.13E-03	6.78E-06
8	-	1.49E-03	1.56E-03	2.19E-04	3.06E-04	1.25E-03	1.15E-05
9	-	1.69E-03	1.56E-03	3.23E-04	2.20E-04	1.33E-03	1.80E-05
10	-	1.88E-03	1.56E-03	4.52E-04	1.63E-04	1.38E-03	2.61E-05
11	-	2.07E-03	1.56E-03	5.96E-04	1.26E-04	1.40E-03	3.51E-05
12	-	2.26E-03	1.56E-03	7.48E-04	1.02E-04	1.42E-03	4.46E-05
13	-	2.44E-03	1.56E-03	9.05E-04	8.44E-05	1.43E-03	5.42E-05
14	-	2.80E-03	1.56E-03	1.22E-03	6.27E-05	1.43E-03	7.32E-05
15	-	3.14E-03	1.56E-03	1.53E-03	4.97E-05	1.42E-03	9.16E-05
16	-	3.79E-03	1.56E-03	2.14E-03	3.52E-05	1.40E-03	1.26E-04
17	-	4.98E-03	1.56E-03	3.25E-03	2.24E-05	1.36E-03	1.85E-04
18	-	6.27E-03	1.56E-03	4.47E-03	1.56E-05	1.30E-03	2.45E-04
19	-	7.38E-03	1.56E-03	5.54E-03	1.22E-05	1.26E-03	2.93E-04
20	-	8.36E-03	1.56E-03	6.47E-03	1.01E-05	1.22E-03	3.32E-04

Measured chemical shifts

Point	pH	S1	D1	D2
1	-	9.45E+00	9.06E+00	8.44E+00
2	-	9.44E+00	9.05E+00	8.43E+00
3	-	9.43E+00	9.03E+00	8.42E+00
4	-	9.41E+00	9.02E+00	8.41E+00
5	-	9.40E+00	9.01E+00	8.40E+00
6	-	9.39E+00	9.00E+00	8.39E+00
7	-	9.38E+00	8.99E+00	8.38E+00
8	-	9.37E+00	8.98E+00	8.37E+00
9	-	9.36E+00	8.98E+00	8.37E+00
10	-	9.36E+00	8.98E+00	8.37E+00

11	-	9.36E+00	8.98E+00	8.36E+00
12	-	9.36E+00	8.98E+00	8.36E+00
13	-	9.36E+00	8.98E+00	8.36E+00
14	-	9.36E+00	8.99E+00	8.36E+00
15	-	9.36E+00	8.99E+00	8.36E+00
16	-	9.36E+00	9.00E+00	8.36E+00
17	-	9.37E+00	9.03E+00	8.37E+00
18	-	9.37E+00	9.05E+00	8.37E+00
19	-	9.37E+00	9.06E+00	8.37E+00
20	-	9.38E+00	9.08E+00	8.37E+00

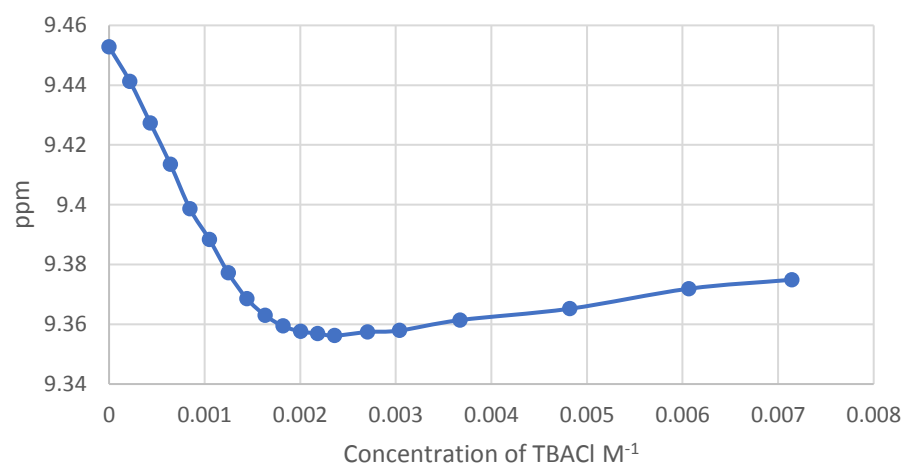
Calculated chemical shifts

Point	pH	S1	D1	D2
1	-	9.46E+00	9.06E+00	8.45E+00
2	-	9.44E+00	9.05E+00	8.43E+00
3	-	9.43E+00	9.03E+00	8.42E+00
4	-	9.41E+00	9.02E+00	8.41E+00
5	-	9.40E+00	9.01E+00	8.40E+00
6	-	9.39E+00	9.00E+00	8.39E+00
7	-	9.38E+00	8.99E+00	8.38E+00
8	-	9.37E+00	8.98E+00	8.37E+00
9	-	9.36E+00	8.98E+00	8.37E+00
10	-	9.36E+00	8.98E+00	8.37E+00
11	-	9.36E+00	8.98E+00	8.36E+00
12	-	9.36E+00	8.98E+00	8.36E+00
13	-	9.36E+00	8.98E+00	8.36E+00
14	-	9.36E+00	8.99E+00	8.36E+00
15	-	9.36E+00	8.99E+00	8.36E+00
16	-	9.36E+00	9.00E+00	8.36E+00
17	-	9.37E+00	9.03E+00	8.37E+00
18	-	9.37E+00	9.05E+00	8.37E+00
19	-	9.38E+00	9.06E+00	8.37E+00
20	-	9.38E+00	9.08E+00	8.37E+00

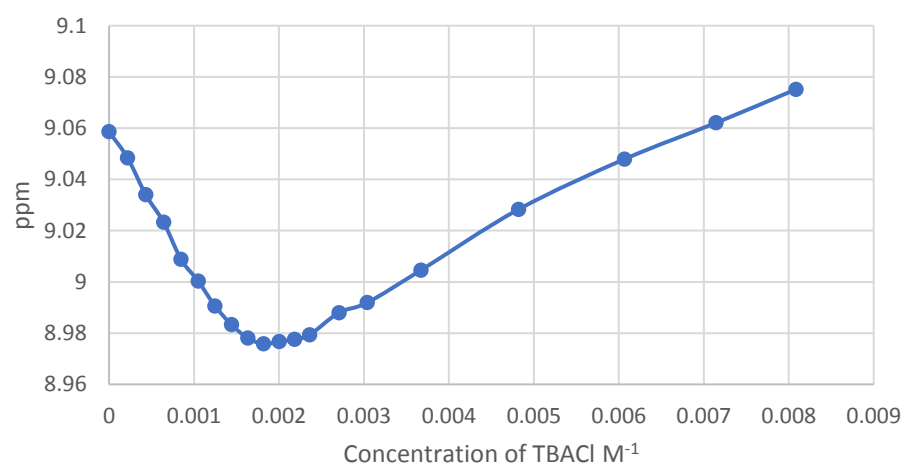
Chemical shifts for each nucleus

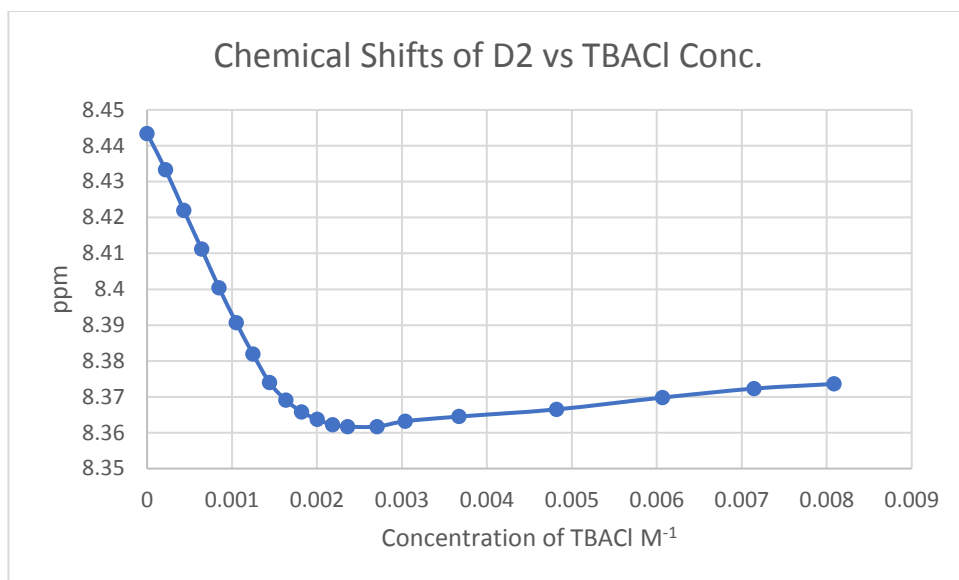
species	S1	D1	D2
H	9.46E+00	9.06E+00	8.45E+00
GH	9.35E+00	8.96E+00	8.36E+00
G ₂ H	9.50E+00	9.52E+00	8.44E+00

Chemical Shifts of S1 vs TBACl Conc.



Chemical Shifts of D1 vs TBACl Conc.





G2XB and TBA⁺Cl⁻ (Experiment 2)

Species	Log beta	G	H	std. dev.
1	4.3459	1	1	0.0795
2	6.1518	2	1	0.0996

Converged in 1 iterations with sigma = 0.140068

Species concentrations/mol dm⁻³

Point	pH	T(TBACl)	T(G2XB)	F(TBACl)	F(G2XB)	species 1	species 2
1	-	0.00E+00	1.51E-03	3.17E-91	1.51E-03	1.06E-89	2.15E-178
2	-	2.16E-04	1.51E-03	7.24E-06	1.30E-03	2.08E-04	9.65E-08
3	-	4.28E-04	1.51E-03	1.68E-05	1.10E-03	4.10E-04	4.42E-07
4	-	6.35E-04	1.51E-03	3.01E-05	9.03E-04	6.03E-04	1.16E-06
5	-	8.39E-04	1.51E-03	4.91E-05	7.20E-04	7.85E-04	2.47E-06
6	-	1.04E-03	1.51E-03	7.78E-05	5.51E-04	9.51E-04	4.73E-06
7	-	1.23E-03	1.51E-03	1.22E-04	4.04E-04	1.09E-03	8.56E-06
8	-	1.43E-03	1.51E-03	1.90E-04	2.86E-04	1.21E-03	1.47E-05
9	-	1.62E-03	1.51E-03	2.86E-04	2.02E-04	1.28E-03	2.35E-05
10	-	1.80E-03	1.51E-03	4.06E-04	1.47E-04	1.33E-03	3.44E-05
11	-	1.98E-03	1.51E-03	5.41E-04	1.12E-04	1.35E-03	4.66E-05
12	-	2.16E-03	1.51E-03	6.84E-04	8.96E-05	1.36E-03	5.94E-05
13	-	2.34E-03	1.51E-03	8.31E-04	7.39E-05	1.36E-03	7.23E-05
14	-	2.68E-03	1.51E-03	1.13E-03	5.42E-05	1.36E-03	9.77E-05
15	-	3.01E-03	1.51E-03	1.42E-03	4.26E-05	1.34E-03	1.22E-04
16	-	3.33E-03	1.51E-03	1.71E-03	3.50E-05	1.33E-03	1.45E-04
17	-	3.63E-03	1.51E-03	1.99E-03	2.97E-05	1.31E-03	1.67E-04
18	-	4.22E-03	1.51E-03	2.53E-03	2.28E-05	1.28E-03	2.07E-04
19	-	5.53E-03	1.51E-03	3.75E-03	1.45E-05	1.20E-03	2.89E-04
20	-	6.87E-03	1.51E-03	5.01E-03	1.02E-05	1.13E-03	3.63E-04

Measured chemical shifts

Point	pH	S1	D1	D2
1	-	9.45E+00	9.06E+00	8.44E+00
2	-	9.44E+00	9.04E+00	8.43E+00
3	-	9.42E+00	9.03E+00	8.42E+00
4	-	9.41E+00	9.02E+00	8.41E+00
5	-	9.39E+00	9.00E+00	8.39E+00
6	-	9.38E+00	8.99E+00	8.38E+00
7	-	9.37E+00	8.98E+00	8.38E+00
8	-	9.36E+00	8.98E+00	8.37E+00
9	-	9.36E+00	8.97E+00	8.36E+00
10	-	9.36E+00	8.97E+00	8.36E+00
11	-	9.36E+00	8.98E+00	8.36E+00
12	-	9.36E+00	8.98E+00	8.36E+00
13	-	9.36E+00	8.98E+00	8.36E+00
14	-	9.36E+00	8.99E+00	8.36E+00
15	-	9.36E+00	8.99E+00	8.36E+00
16	-	9.36E+00	9.00E+00	8.36E+00
17	-	9.36E+00	9.01E+00	8.36E+00
18	-	9.36E+00	9.02E+00	8.36E+00
19	-	9.37E+00	9.04E+00	8.37E+00
20	-	9.37E+00	9.06E+00	8.37E+00

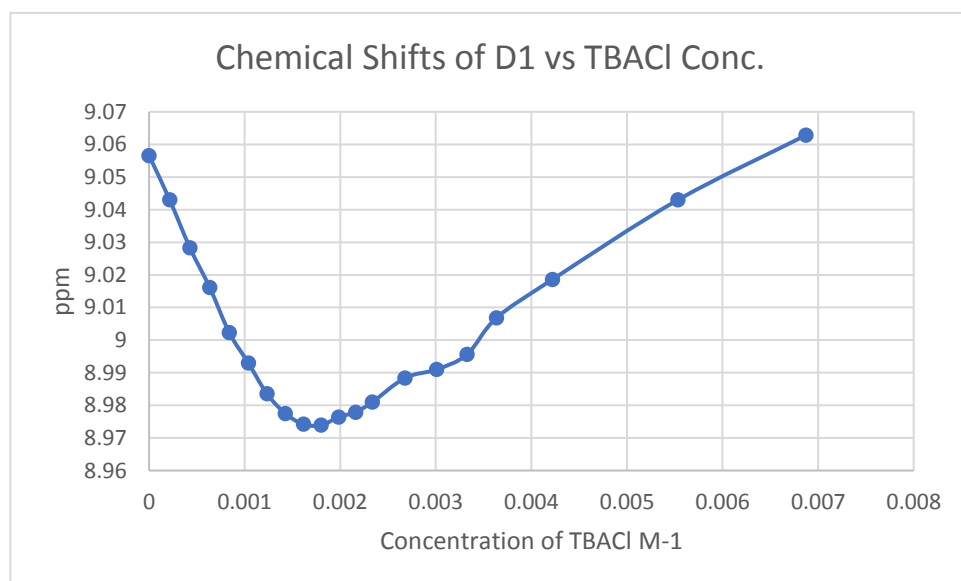
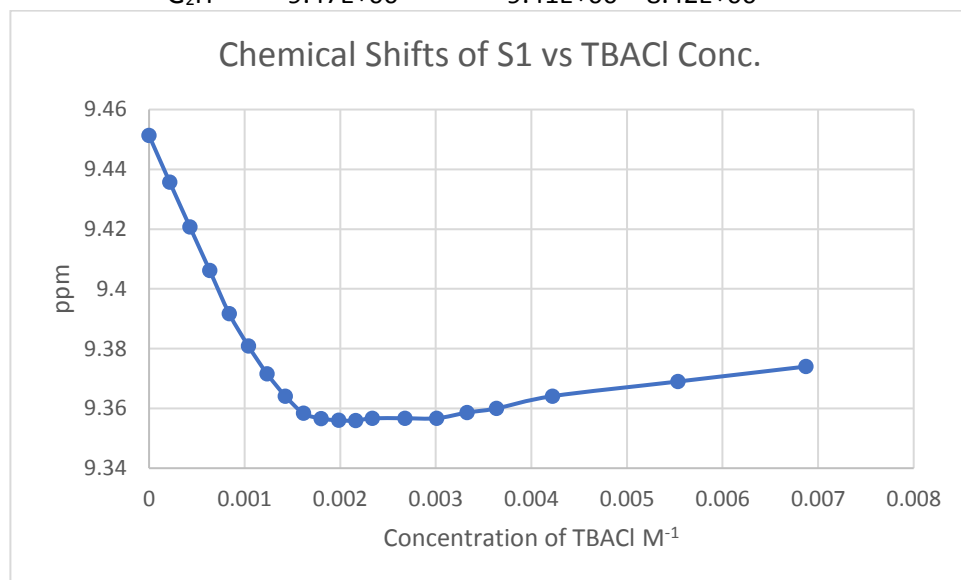
Calculated chemical shifts

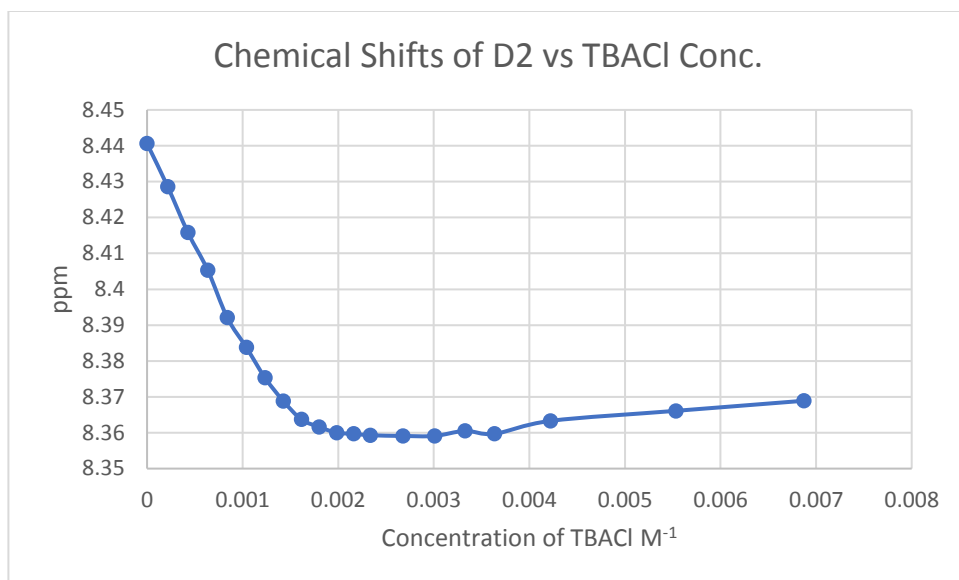
Point	pH	S1	D1	D2
1	-	9.45E+00	9.06E+00	8.44E+00
2	-	9.43E+00	9.04E+00	8.43E+00
3	-	9.42E+00	9.03E+00	8.42E+00
4	-	9.41E+00	9.02E+00	8.40E+00
5	-	9.39E+00	9.00E+00	8.39E+00
6	-	9.38E+00	8.99E+00	8.38E+00
7	-	9.37E+00	8.98E+00	8.38E+00
8	-	9.36E+00	8.98E+00	8.37E+00
9	-	9.36E+00	8.97E+00	8.36E+00
10	-	9.36E+00	8.97E+00	8.36E+00
11	-	9.36E+00	8.98E+00	8.36E+00
12	-	9.35E+00	8.98E+00	8.36E+00
13	-	9.35E+00	8.98E+00	8.36E+00
14	-	9.36E+00	8.99E+00	8.36E+00
15	-	9.36E+00	8.99E+00	8.36E+00
16	-	9.36E+00	9.00E+00	8.36E+00
17	-	9.36E+00	9.01E+00	8.36E+00
18	-	9.36E+00	9.02E+00	8.36E+00

19	-	9.37E+00	9.04E+00	8.37E+00
20	-	9.38E+00	9.06E+00	8.37E+00

Chemical shifts for each nucleus

species	S1	D1	D2
H	9.45E+00	9.06E+00	8.44E+00
GH	9.34E+00	8.95E+00	8.35E+00
G ₂ H	9.47E+00	9.41E+00	8.42E+00





G2XB and TBA⁺Cl⁻ (Experiment 3)

Species	Log beta	G	H	std. dev.
1	4.5046	1	1	0.0491
2	6.3786	2	1	0.053

Converged in 1 iterations with sigma = 0.078751

Species concentrations/mol dm⁻³

Point	pH	T(TBACl)	T(G2XB)	F(TBACl)	F(G2XB)	species 1	species 2
1	-	0.00E+00	1.51E-03	2.71E-91	1.51E-03	1.30E-89	2.64E-178
2	-	2.16E-04	1.51E-03	5.08E-06	1.30E-03	2.11E-04	8.01E-08
3	-	4.28E-04	1.51E-03	1.19E-05	1.09E-03	4.15E-04	3.69E-07
4	-	6.35E-04	1.51E-03	2.14E-05	8.94E-04	6.12E-04	9.80E-07
5	-	8.39E-04	1.51E-03	3.54E-05	7.06E-04	7.99E-04	2.12E-06
6	-	1.04E-03	1.51E-03	5.74E-05	5.30E-04	9.73E-04	4.18E-06
7	-	1.23E-03	1.51E-03	9.39E-05	3.75E-04	1.12E-03	7.90E-06
8	-	1.43E-03	1.51E-03	1.55E-04	2.50E-04	1.24E-03	1.44E-05
9	-	1.62E-03	1.51E-03	2.49E-04	1.65E-04	1.32E-03	2.45E-05
10	-	1.80E-03	1.51E-03	3.70E-04	1.15E-04	1.36E-03	3.75E-05
11	-	1.98E-03	1.51E-03	5.08E-04	8.45E-05	1.37E-03	5.21E-05
12	-	2.16E-03	1.51E-03	6.53E-04	6.59E-05	1.37E-03	6.71E-05
13	-	2.34E-03	1.51E-03	8.01E-04	5.36E-05	1.37E-03	8.22E-05
14	-	2.68E-03	1.51E-03	1.10E-03	3.87E-05	1.36E-03	1.11E-04
15	-	3.01E-03	1.51E-03	1.39E-03	3.01E-05	1.34E-03	1.39E-04
16	-	3.33E-03	1.51E-03	1.68E-03	2.46E-05	1.32E-03	1.65E-04
17	-	3.63E-03	1.51E-03	1.96E-03	2.07E-05	1.30E-03	1.90E-04
18	-	4.22E-03	1.51E-03	2.49E-03	1.58E-05	1.26E-03	2.35E-04
19	-	5.53E-03	1.51E-03	3.71E-03	9.88E-06	1.17E-03	3.25E-04

20	-	6.87E-03	1.51E-03	4.96E-03	6.90E-06	1.09E-03	4.06E-04
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Measured chemical shifts

Point	pH	S1	D1	D2
1	-	9.45E+00	9.06E+00	8.44E+00
2	-	9.44E+00	9.04E+00	8.43E+00
3	-	9.42E+00	9.03E+00	8.42E+00
4	-	9.41E+00	9.02E+00	8.40E+00
5	-	9.39E+00	9.00E+00	8.40E+00
6	-	9.38E+00	8.99E+00	8.38E+00
7	-	9.37E+00	8.98E+00	8.38E+00
8	-	9.36E+00	8.98E+00	8.37E+00
9	-	9.36E+00	8.97E+00	8.37E+00
10	-	9.36E+00	8.98E+00	8.36E+00
11	-	9.36E+00	8.98E+00	8.36E+00
12	-	9.36E+00	8.98E+00	8.36E+00
13	-	9.36E+00	8.98E+00	8.36E+00
14	-	9.36E+00	8.99E+00	8.36E+00
15	-	9.36E+00	8.99E+00	8.36E+00
16	-	9.36E+00	9.00E+00	8.36E+00
17	-	9.36E+00	9.01E+00	8.36E+00
18	-	9.36E+00	9.02E+00	8.36E+00
19	-	9.37E+00	9.04E+00	8.37E+00
20	-	9.37E+00	9.06E+00	8.37E+00

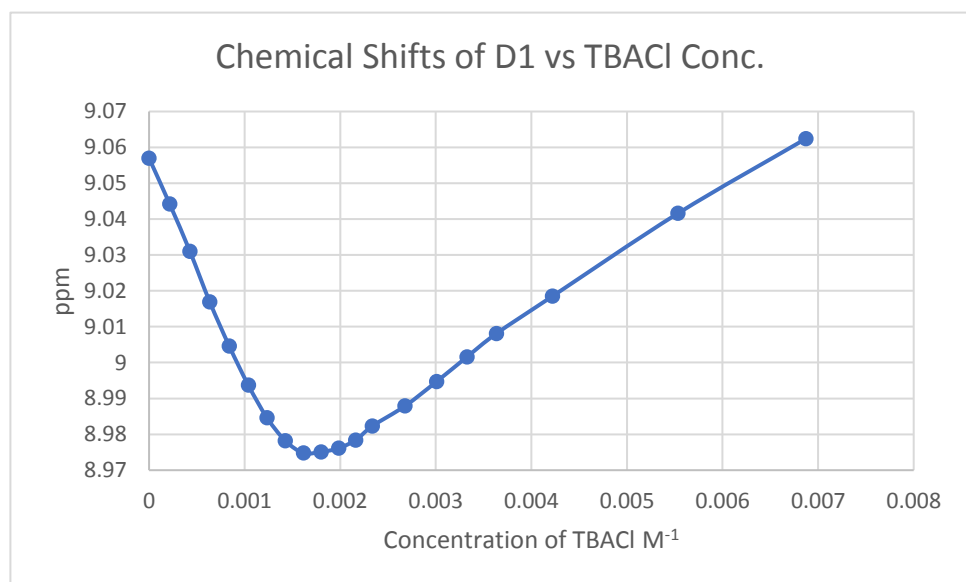
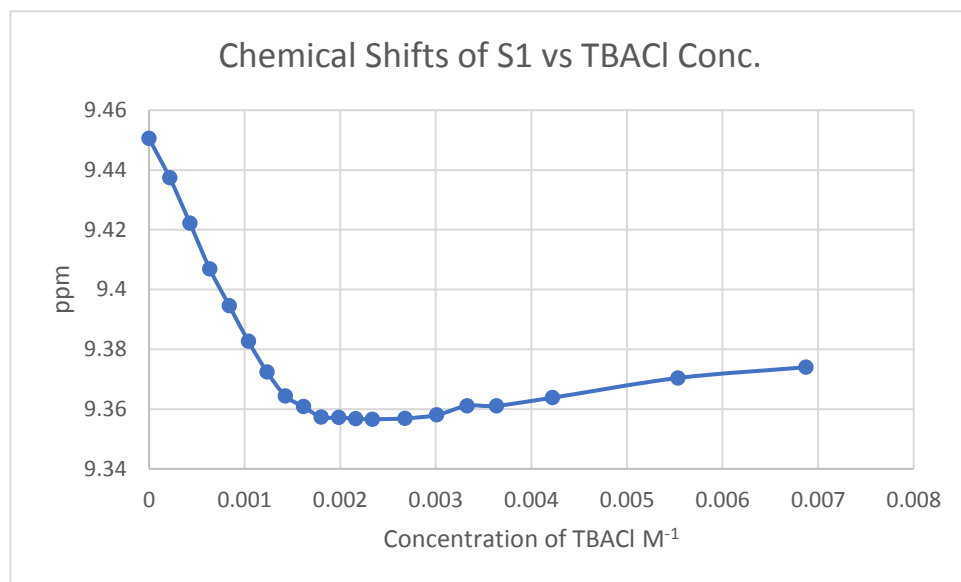
Calculated chemical shifts

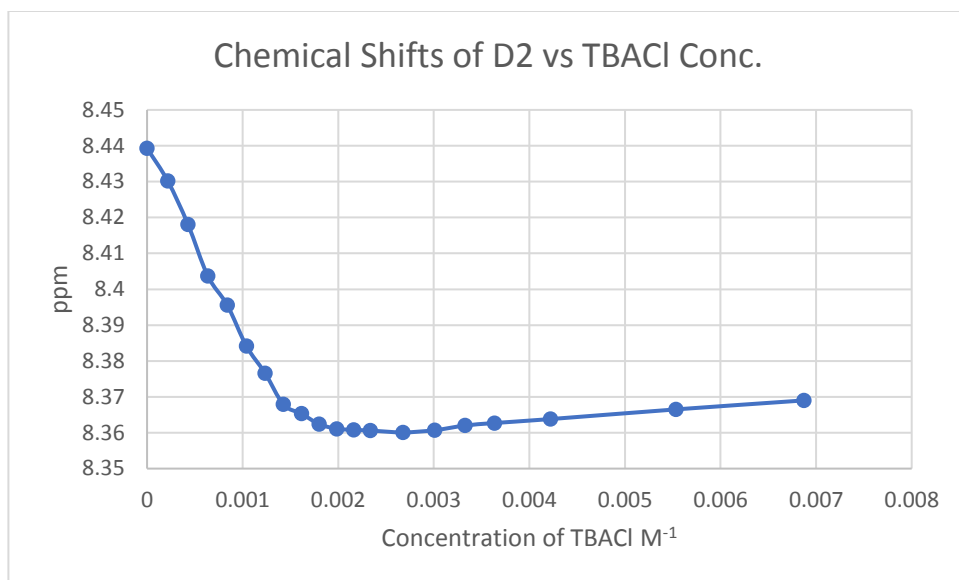
Point	pH	S1	D1	D2
1	-	9.45E+00	9.06E+00	8.44E+00
2	-	9.44E+00	9.04E+00	8.43E+00
3	-	9.42E+00	9.03E+00	8.42E+00
4	-	9.41E+00	9.02E+00	8.41E+00
5	-	9.40E+00	9.00E+00	8.39E+00
6	-	9.38E+00	8.99E+00	8.38E+00
7	-	9.37E+00	8.98E+00	8.38E+00
8	-	9.37E+00	8.98E+00	8.37E+00
9	-	9.36E+00	8.97E+00	8.36E+00
10	-	9.36E+00	8.97E+00	8.36E+00
11	-	9.36E+00	8.98E+00	8.36E+00
12	-	9.36E+00	8.98E+00	8.36E+00
13	-	9.36E+00	8.98E+00	8.36E+00
14	-	9.36E+00	8.99E+00	8.36E+00
15	-	9.36E+00	9.00E+00	8.36E+00
16	-	9.36E+00	9.00E+00	8.36E+00
17	-	9.36E+00	9.01E+00	8.36E+00

18	-	9.36E+00	9.02E+00	8.36E+00
19	-	9.37E+00	9.04E+00	8.37E+00
20	-	9.38E+00	9.06E+00	8.37E+00

Chemical shifts for each nucleus

species	S1	D1	D2
H	9.45E+00	9.06E+00	8.44E+00
GH	9.35E+00	8.96E+00	8.35E+00
G ₂ H	9.45E+00	9.34E+00	8.41E+00





G2XB and TBA⁺Br⁻ (Experiment 1)

Species	Log beta	G	H	std. dev.
1	4.4065	1	1	0.1095
2	6.8151	2	1	0.1048

Converged in 1 iterations with sigma = 0.217308

Species concentrations/mol dm⁻³

Point	pH	T(TBABr)	T(G2XB)	F(TBABr)	F(G2XB)	species 1	species 2
1	-	0.00E+00	1.60E-03	3.02E-91	1.60E-03	1.23E-89	9.51E-178
2	-	1.70E-04	1.60E-03	4.52E-06	1.43E-03	1.65E-04	1.91E-07
3	-	3.36E-04	1.60E-03	1.00E-05	1.27E-03	3.24E-04	8.32E-07
4	-	4.99E-04	1.60E-03	1.68E-05	1.12E-03	4.78E-04	2.06E-06
5	-	6.59E-04	1.60E-03	2.54E-05	9.66E-04	6.25E-04	4.07E-06
6	-	8.16E-04	1.60E-03	3.64E-05	8.23E-04	7.65E-04	7.14E-06
7	-	9.70E-04	1.60E-03	5.10E-05	6.88E-04	8.95E-04	1.17E-05
8	-	1.12E-03	1.60E-03	7.05E-05	5.64E-04	1.01E-03	1.83E-05
9	-	1.27E-03	1.60E-03	9.70E-05	4.51E-04	1.12E-03	2.78E-05
10	-	1.41E-03	1.60E-03	1.33E-04	3.55E-04	1.20E-03	4.08E-05
11	-	1.56E-03	1.60E-03	1.80E-04	2.76E-04	1.26E-03	5.80E-05
12	-	1.70E-03	1.60E-03	2.38E-04	2.15E-04	1.30E-03	7.93E-05
13	-	1.84E-03	1.60E-03	3.06E-04	1.70E-04	1.32E-03	1.04E-04
14	-	2.10E-03	1.60E-03	4.63E-04	1.12E-04	1.33E-03	1.57E-04
15	-	2.36E-03	1.60E-03	6.36E-04	8.04E-05	1.30E-03	2.12E-04
16	-	2.86E-03	1.60E-03	9.94E-04	4.86E-05	1.23E-03	3.14E-04
17	-	3.32E-03	1.60E-03	1.35E-03	3.36E-05	1.16E-03	4.02E-04
18	-	5.23E-03	1.60E-03	2.97E-03	1.19E-05	9.00E-04	6.84E-04
19	-	6.69E-03	1.60E-03	4.27E-03	6.97E-06	7.59E-04	8.30E-04
20	-	8.30E-03	1.60E-03	5.76E-03	4.37E-06	6.43E-04	9.48E-04

Measured chemical shifts

Point	pH	S1	D1	D2
1	-	9.45E+00	9.06E+00	8.44E+00
2	-	9.44E+00	9.05E+00	8.43E+00
3	-	9.43E+00	9.04E+00	8.42E+00
4	-	9.41E+00	9.03E+00	8.41E+00
5	-	9.40E+00	9.02E+00	8.41E+00
6	-	9.39E+00	9.01E+00	8.40E+00
7	-	9.38E+00	9.00E+00	8.39E+00
8	-	9.37E+00	8.99E+00	8.38E+00
9	-	9.37E+00	8.99E+00	8.38E+00
10	-	9.36E+00	8.98E+00	8.37E+00
11	-	9.36E+00	8.98E+00	8.37E+00
12	-	9.35E+00	8.98E+00	8.37E+00
13	-	9.35E+00	8.98E+00	8.37E+00
14	-	9.35E+00	8.98E+00	8.37E+00
15	-	9.35E+00	8.99E+00	8.37E+00
16	-	9.35E+00	8.99E+00	8.37E+00
17	-	9.36E+00	9.00E+00	8.37E+00
18	-	9.37E+00	9.03E+00	8.37E+00
19	-	9.37E+00	9.05E+00	8.38E+00
20	-	9.38E+00	9.07E+00	8.38E+00

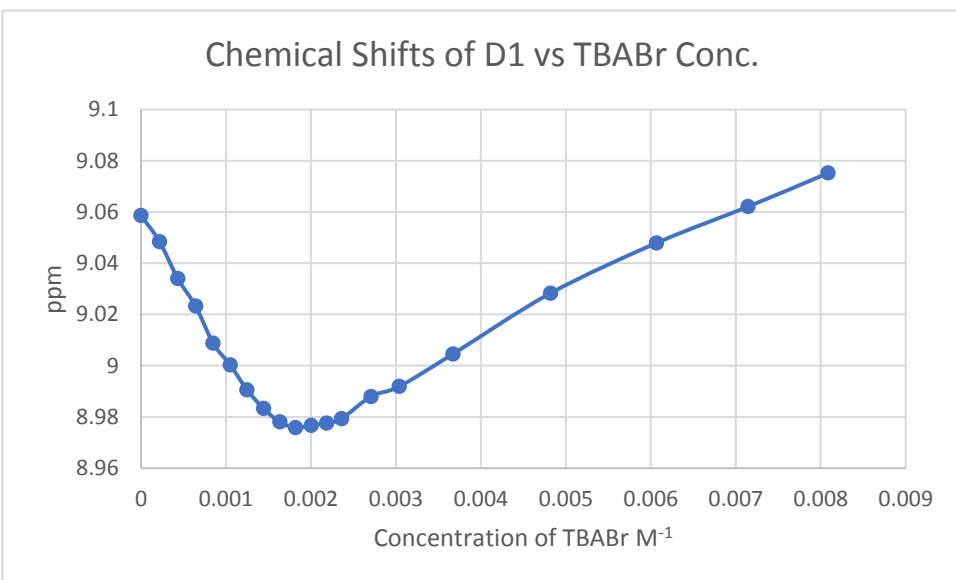
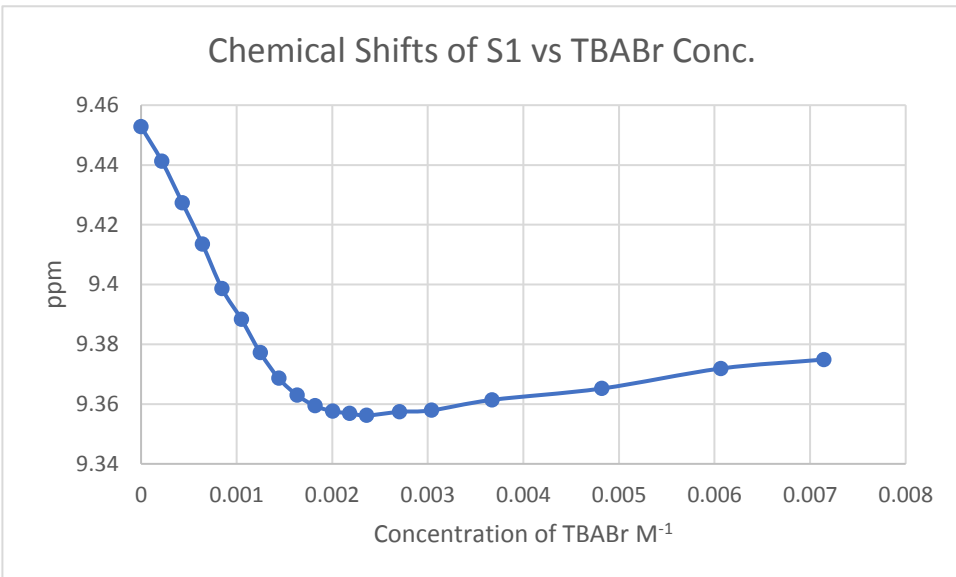
Calculated chemical shifts

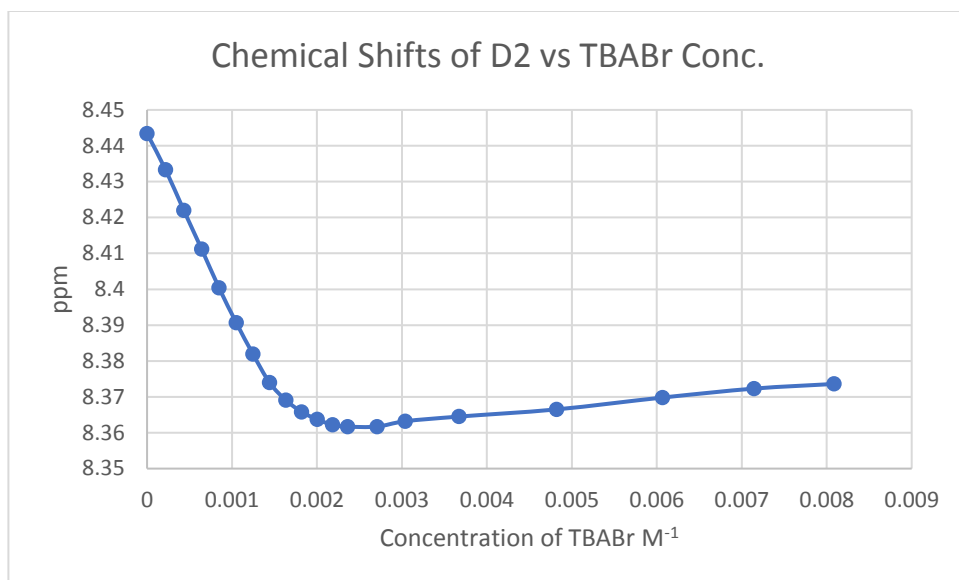
Point	pH	S1	D1	D2
1	-	9.45E+00	9.06E+00	8.44E+00
2	-	9.44E+00	9.05E+00	8.43E+00
3	-	9.43E+00	9.04E+00	8.42E+00
4	-	9.42E+00	9.03E+00	8.42E+00
5	-	9.40E+00	9.02E+00	8.41E+00
6	-	9.39E+00	9.01E+00	8.40E+00
7	-	9.39E+00	9.00E+00	8.39E+00
8	-	9.38E+00	8.99E+00	8.39E+00
9	-	9.37E+00	8.99E+00	8.38E+00
10	-	9.36E+00	8.98E+00	8.37E+00
11	-	9.36E+00	8.98E+00	8.37E+00
12	-	9.35E+00	8.98E+00	8.37E+00
13	-	9.35E+00	8.98E+00	8.37E+00
14	-	9.35E+00	8.98E+00	8.36E+00
15	-	9.35E+00	8.98E+00	8.36E+00
16	-	9.35E+00	8.99E+00	8.37E+00
17	-	9.36E+00	9.00E+00	8.37E+00
18	-	9.37E+00	9.04E+00	8.38E+00

19	-	9.37E+00	9.05E+00	8.38E+00
20	-	9.38E+00	9.07E+00	8.38E+00

Chemical shifts for each nucleus

species	S1	D1	D2
H	9.45E+00	9.06E+00	8.44E+00
GH	9.33E+00	8.95E+00	8.35E+00
G ₂ H	9.41E+00	9.15E+00	8.40E+00





G2XB and TBA⁺Br⁻ (Experiment 2)

Species	Log beta	G	H	std. dev.
1	4.4892	1	1	0.1549
2	7.1182	2	1	0.1324

Converged in 1 iterations with sigma = 0.293553

Species concentrations/mol dm⁻³

Point	pH	T(TBABr)	T(G2XB)	F(TBABr)	F(G2XB)	species 1	species 2
1	-	0.00E+00	1.51E-03	2.78E-91	1.51E-03	1.29E-89	1.53E-177
2	-	2.33E-04	1.51E-03	5.72E-06	1.28E-03	2.26E-04	5.49E-07
3	-	4.61E-04	1.51E-03	1.35E-05	1.06E-03	4.42E-04	2.54E-06
4	-	6.84E-04	1.51E-03	2.45E-05	8.54E-04	6.46E-04	6.75E-06
5	-	9.04E-04	1.51E-03	4.10E-05	6.59E-04	8.34E-04	1.46E-05
6	-	1.12E-03	1.51E-03	6.68E-05	4.83E-04	9.96E-04	2.83E-05
7	-	1.33E-03	1.51E-03	1.08E-04	3.36E-04	1.12E-03	5.14E-05
8	-	1.54E-03	1.51E-03	1.71E-04	2.27E-04	1.19E-03	8.66E-05
9	-	1.74E-03	1.51E-03	2.56E-04	1.55E-04	1.22E-03	1.33E-04
10	-	1.94E-03	1.51E-03	3.58E-04	1.10E-04	1.21E-03	1.85E-04
11	-	2.14E-03	1.51E-03	4.72E-04	8.15E-05	1.19E-03	2.39E-04
12	-	2.33E-03	1.51E-03	5.93E-04	6.30E-05	1.15E-03	2.91E-04
13	-	2.52E-03	1.51E-03	7.19E-04	5.03E-05	1.12E-03	3.42E-04
14	-	2.89E-03	1.51E-03	9.80E-04	3.44E-05	1.04E-03	4.33E-04
15	-	3.24E-03	1.51E-03	1.25E-03	2.52E-05	9.69E-04	5.14E-04
16	-	3.58E-03	1.51E-03	1.51E-03	1.94E-05	9.05E-04	5.83E-04
17	-	3.92E-03	1.51E-03	1.78E-03	1.54E-05	8.48E-04	6.43E-04
18	-	4.55E-03	1.51E-03	2.31E-03	1.06E-05	7.55E-04	7.42E-04
19	-	5.96E-03	1.51E-03	3.56E-03	5.45E-06	5.97E-04	9.04E-04
20	-	7.40E-03	1.51E-03	4.88E-03	3.24E-06	4.89E-04	1.02E-03

Measured chemical shifts

Point	pH	S1	D1	D2
1	-	9.45E+00	9.06E+00	8.44E+00
2	-	9.43E+00	9.04E+00	8.42E+00
3	-	9.41E+00	9.02E+00	8.41E+00
4	-	9.39E+00	9.01E+00	8.40E+00
5	-	9.38E+00	8.99E+00	8.39E+00
6	-	9.36E+00	8.98E+00	8.38E+00
7	-	9.36E+00	8.98E+00	8.37E+00
8	-	9.35E+00	8.97E+00	8.37E+00
9	-	9.35E+00	8.98E+00	8.37E+00
10	-	9.35E+00	8.98E+00	8.37E+00
11	-	9.35E+00	8.98E+00	8.37E+00
12	-	9.35E+00	8.99E+00	8.37E+00
13	-	9.35E+00	8.99E+00	8.37E+00
14	-	9.35E+00	9.00E+00	8.37E+00
15	-	9.36E+00	9.01E+00	8.37E+00
16	-	9.36E+00	9.01E+00	8.37E+00
17	-	9.36E+00	9.02E+00	8.37E+00
18	-	9.36E+00	9.03E+00	8.37E+00
19	-	9.37E+00	9.05E+00	8.38E+00
20	-	9.37E+00	9.06E+00	8.38E+00

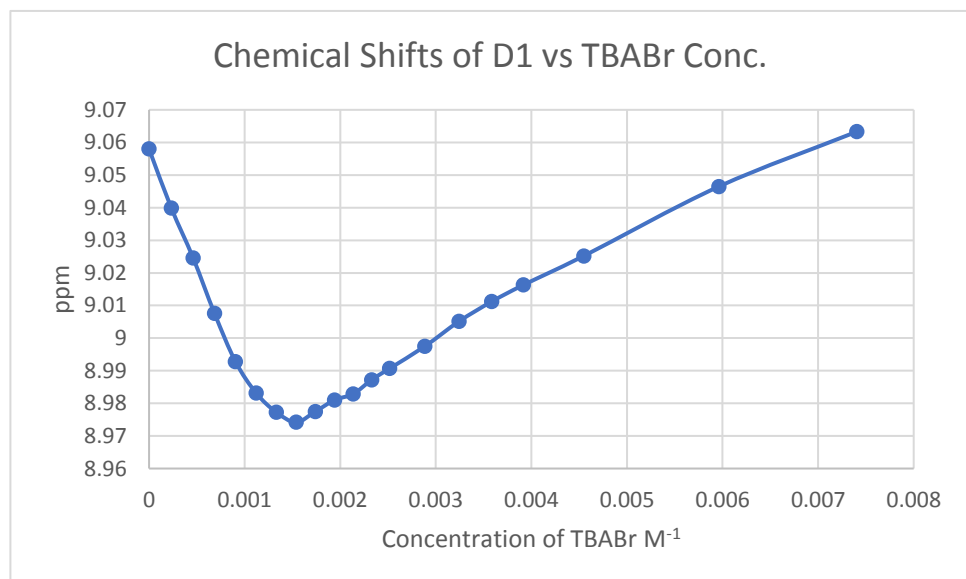
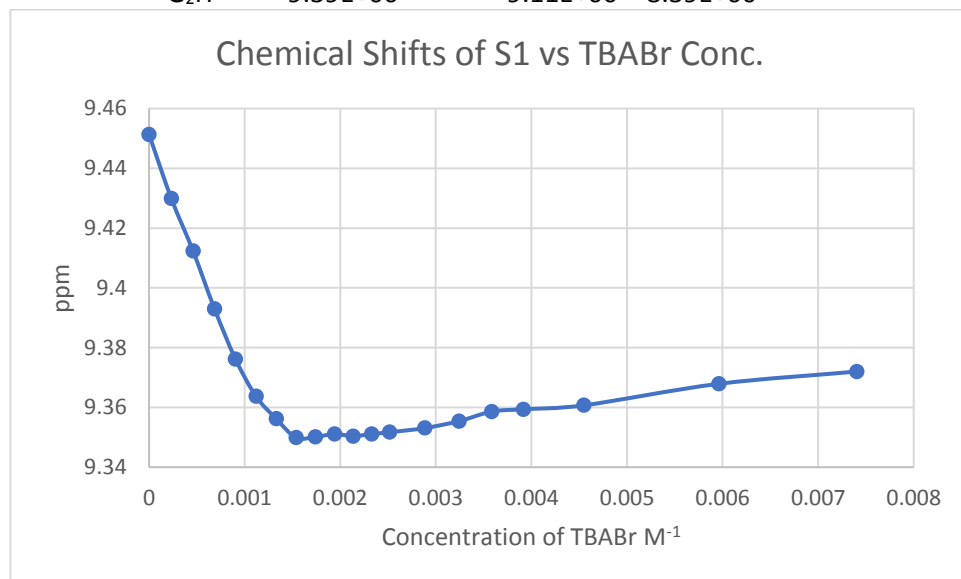
Calculated chemical shifts

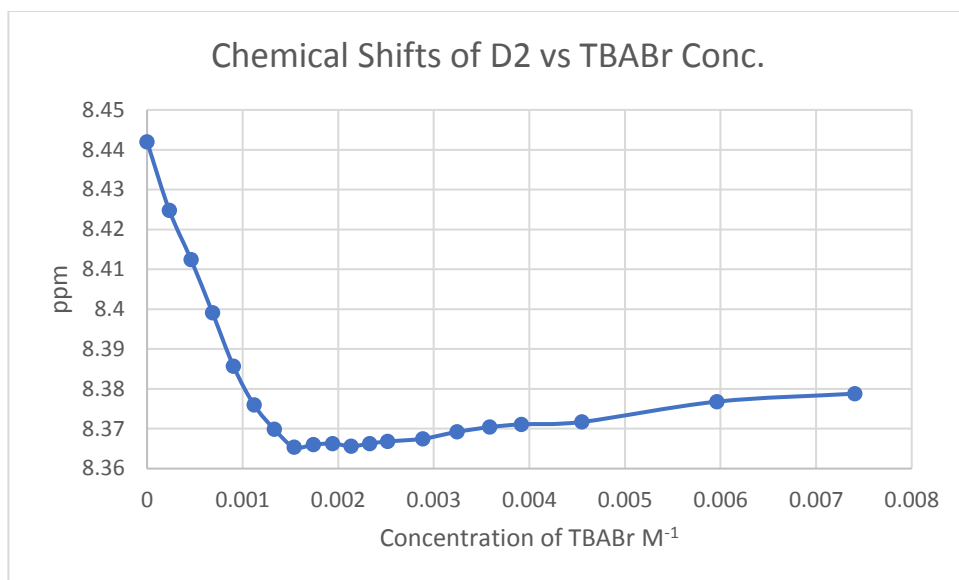
Point	pH	S1	D1	D2
1	-	9.45E+00	9.06E+00	8.44E+00
2	-	9.43E+00	9.04E+00	8.42E+00
3	-	9.41E+00	9.02E+00	8.41E+00
4	-	9.40E+00	9.01E+00	8.40E+00
5	-	9.38E+00	9.00E+00	8.39E+00
6	-	9.37E+00	8.99E+00	8.38E+00
7	-	9.36E+00	8.98E+00	8.37E+00
8	-	9.35E+00	8.97E+00	8.37E+00
9	-	9.35E+00	8.97E+00	8.36E+00
10	-	9.35E+00	8.98E+00	8.36E+00
11	-	9.35E+00	8.98E+00	8.36E+00
12	-	9.35E+00	8.98E+00	8.36E+00
13	-	9.35E+00	8.99E+00	8.36E+00
14	-	9.35E+00	9.00E+00	8.37E+00
15	-	9.35E+00	9.01E+00	8.37E+00
16	-	9.36E+00	9.01E+00	8.37E+00
17	-	9.36E+00	9.02E+00	8.37E+00

18	-	9.36E+00	9.03E+00	8.37E+00
19	-	9.37E+00	9.05E+00	8.38E+00
20	-	9.37E+00	9.06E+00	8.38E+00

Chemical shifts for each nucleus

species	S1	D1	D2
H	9.45E+00	9.06E+00	8.44E+00
GH	9.33E+00	8.95E+00	8.35E+00
G ₂ H	9.39E+00	9.11E+00	8.39E+00





G2XB and TBA⁺Br⁻ (Experiment 3)

Species	Log beta	G	H	std. dev.
				0.1246
1	4.6554	1	1	fa
2	7.0062	2	1	0.1022

Converged in 1 iterations with sigma = 0.192988

Species concentrations/mol dm⁻³

Point	pH	T(TBABr)	T(G2XB)	F(TBABr)	F(G2XB)	species 1	species 2
1	-	0.00E+00	1.51E-03	2.39E-91	1.51E-03	1.63E-89	8.74E-178
2	-	2.33E-04	1.51E-03	3.95E-06	1.28E-03	2.28E-04	2.02E-07
3	-	4.61E-04	1.51E-03	9.40E-06	1.06E-03	4.49E-04	9.48E-07
4	-	6.84E-04	1.51E-03	1.74E-05	8.43E-04	6.62E-04	2.58E-06
5	-	9.04E-04	1.51E-03	2.98E-05	6.39E-04	8.62E-04	5.77E-06
6	-	1.12E-03	1.51E-03	5.11E-05	4.51E-04	1.04E-03	1.20E-05
7	-	1.33E-03	1.51E-03	9.04E-05	2.92E-04	1.19E-03	2.41E-05
8	-	1.54E-03	1.51E-03	1.61E-04	1.77E-04	1.28E-03	4.63E-05
9	-	1.74E-03	1.51E-03	2.65E-04	1.10E-04	1.32E-03	7.84E-05
10	-	1.94E-03	1.51E-03	3.92E-04	7.43E-05	1.32E-03	1.16E-04
11	-	2.14E-03	1.51E-03	5.29E-04	5.43E-05	1.30E-03	1.54E-04
12	-	2.33E-03	1.51E-03	6.72E-04	4.19E-05	1.27E-03	1.92E-04
13	-	2.52E-03	1.51E-03	8.16E-04	3.37E-05	1.25E-03	2.28E-04
14	-	2.89E-03	1.51E-03	1.11E-03	2.37E-05	1.19E-03	2.95E-04
15	-	3.24E-03	1.51E-03	1.40E-03	1.80E-05	1.13E-03	3.55E-04
16	-	3.58E-03	1.51E-03	1.68E-03	1.42E-05	1.08E-03	4.09E-04
17	-	3.92E-03	1.51E-03	1.96E-03	1.17E-05	1.04E-03	4.57E-04
18	-	4.55E-03	1.51E-03	2.51E-03	8.45E-06	9.59E-04	5.40E-04

19	-	5.96E-03	1.51E-03	3.77E-03	4.77E-06	8.14E-04	6.89E-04
20	-	7.40E-03	1.51E-03	5.10E-03	3.04E-06	7.02E-04	8.02E-04

Measured chemical shifts

Point	pH	S1	D1	D2
1	-	9.45E+00	9.06E+00	8.44E+00
2	-	9.43E+00	9.04E+00	8.43E+00
3	-	9.42E+00	9.03E+00	8.42E+00
4	-	9.40E+00	9.01E+00	8.40E+00
5	-	9.38E+00	9.00E+00	8.39E+00
6	-	9.37E+00	8.99E+00	8.38E+00
7	-	9.36E+00	8.98E+00	8.37E+00
8	-	9.35E+00	8.98E+00	8.37E+00
9	-	9.35E+00	8.98E+00	8.37E+00
10	-	9.35E+00	8.98E+00	8.37E+00
11	-	9.35E+00	8.98E+00	8.37E+00
12	-	9.35E+00	8.99E+00	8.37E+00
13	-	9.35E+00	8.99E+00	8.37E+00
14	-	9.35E+00	9.00E+00	8.37E+00
15	-	9.36E+00	9.00E+00	8.37E+00
16	-	9.36E+00	9.01E+00	8.37E+00
17	-	9.36E+00	9.02E+00	8.37E+00
18	-	9.36E+00	9.03E+00	8.37E+00
19	-	9.37E+00	9.05E+00	8.38E+00
20	-	9.37E+00	9.06E+00	8.38E+00

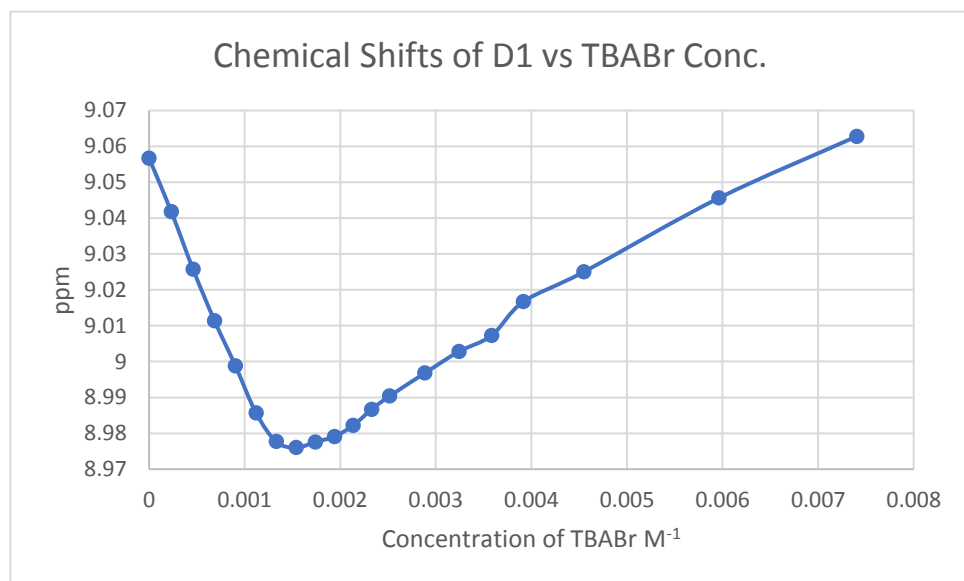
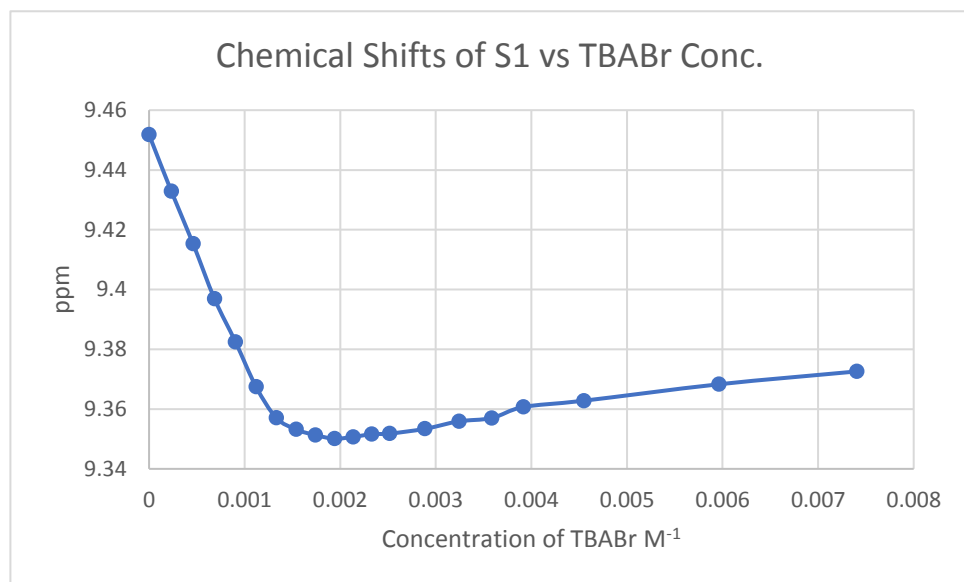
Calculated chemical shifts

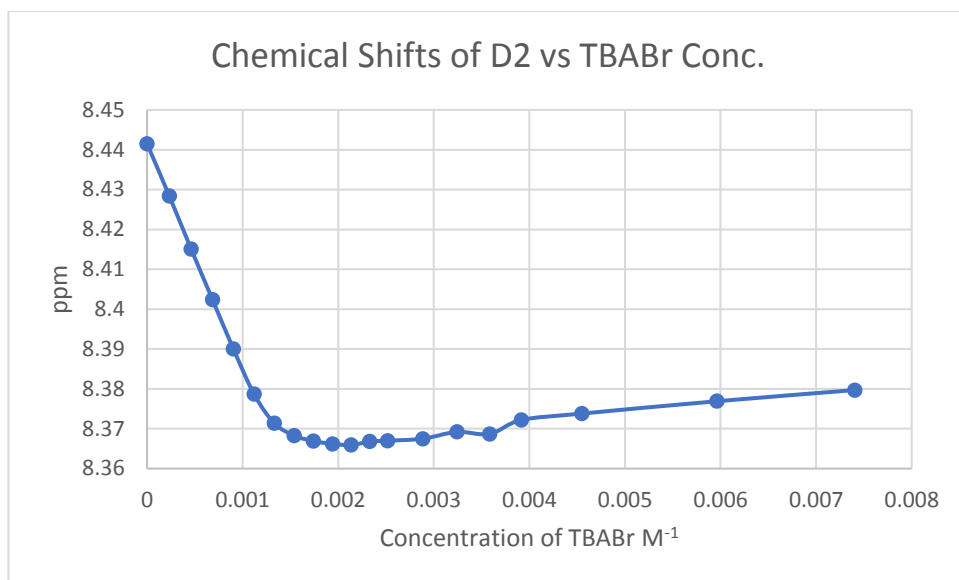
Point	pH	S1	D1	D2
1	-	9.45E+00	9.06E+00	8.44E+00
2	-	9.43E+00	9.04E+00	8.43E+00
3	-	9.42E+00	9.03E+00	8.42E+00
4	-	9.40E+00	9.01E+00	8.40E+00
5	-	9.39E+00	9.00E+00	8.39E+00
6	-	9.37E+00	8.99E+00	8.38E+00
7	-	9.36E+00	8.98E+00	8.37E+00
8	-	9.35E+00	8.98E+00	8.37E+00
9	-	9.35E+00	8.97E+00	8.37E+00
10	-	9.35E+00	8.98E+00	8.36E+00
11	-	9.35E+00	8.98E+00	8.36E+00
12	-	9.35E+00	8.98E+00	8.37E+00
13	-	9.35E+00	8.99E+00	8.37E+00
14	-	9.35E+00	9.00E+00	8.37E+00
15	-	9.36E+00	9.00E+00	8.37E+00

16	-	9.36E+00	9.01E+00	8.37E+00
17	-	9.36E+00	9.02E+00	8.37E+00
18	-	9.36E+00	9.03E+00	8.37E+00
19	-	9.37E+00	9.05E+00	8.38E+00
20	-	9.37E+00	9.06E+00	8.38E+00

Chemical shifts for each nucleus

species	S1	D1	D2
H	9.45E+00	9.06E+00	8.44E+00
GH	9.34E+00	8.96E+00	8.36E+00
G ₂ H	9.41E+00	9.15E+00	8.40E+00





G2XB and TBA⁺I⁻ (Experiment 1)

Species	Log beta	G	H	std. dev.
				0.0565
1	4.4244	1	1	
				0.085
2	6.2373	2	1	

Converged in 1 iterations with sigma = 0.090835

Species concentrations/mol dm⁻³

Point	pH	T(TBAI)	T(G2XB)	F(TBAI)	F(G2XB)	species 1	species 2
1	-	0.00E+00	1.60E-03	2.95E-91	1.60E-03	1.26E-89	2.42E-178
2	-	2.30E-04	1.60E-03	6.09E-06	1.38E-03	2.23E-04	8.85E-08
3	-	4.55E-04	1.60E-03	1.42E-05	1.16E-03	4.40E-04	4.07E-07
4	-	6.76E-04	1.60E-03	2.55E-05	9.55E-04	6.48E-04	1.08E-06
5	-	8.93E-04	1.60E-03	4.21E-05	7.56E-04	8.46E-04	2.31E-06
6	-	1.11E-03	1.60E-03	6.77E-05	5.72E-04	1.03E-03	4.52E-06
7	-	1.31E-03	1.60E-03	1.09E-04	4.09E-04	1.19E-03	8.43E-06
8	-	1.52E-03	1.60E-03	1.77E-04	2.79E-04	1.31E-03	1.51E-05
9	-	1.72E-03	1.60E-03	2.78E-04	1.89E-04	1.39E-03	2.51E-05
10	-	1.92E-03	1.60E-03	4.06E-04	1.33E-04	1.43E-03	3.79E-05
11	-	2.11E-03	1.60E-03	5.52E-04	9.91E-05	1.45E-03	5.21E-05
12	-	2.30E-03	1.60E-03	7.06E-04	7.78E-05	1.46E-03	6.70E-05
13	-	2.49E-03	1.60E-03	8.63E-04	6.36E-05	1.46E-03	8.19E-05
14	-	2.85E-03	1.60E-03	1.18E-03	4.62E-05	1.45E-03	1.11E-04
15	-	3.20E-03	1.60E-03	1.49E-03	3.60E-05	1.43E-03	1.39E-04
16	-	3.87E-03	1.60E-03	2.10E-03	2.49E-05	1.39E-03	1.90E-04
17	-	5.08E-03	1.60E-03	3.21E-03	1.54E-05	1.31E-03	2.75E-04

18	-	6.39E-03	1.60E-03	4.44E-03	1.05E-05	1.24E-03	3.57E-04
19	-	7.53E-03	1.60E-03	5.51E-03	8.03E-06	1.18E-03	4.21E-04
20	-	8.52E-03	1.60E-03	6.45E-03	6.57E-06	1.13E-03	4.72E-04

Measured chemical shifts

Point	pH	S1	D1	D2
1	-	9.46E+00	9.06E+00	8.44E+00
2	-	9.44E+00	9.05E+00	8.44E+00
3	-	9.42E+00	9.04E+00	8.43E+00
4	-	9.41E+00	9.03E+00	8.42E+00
5	-	9.39E+00	9.01E+00	8.41E+00
6	-	9.38E+00	9.01E+00	8.40E+00
7	-	9.37E+00	9.00E+00	8.39E+00
8	-	9.36E+00	8.99E+00	8.39E+00
9	-	9.35E+00	8.99E+00	8.38E+00
10	-	9.35E+00	8.99E+00	8.38E+00
11	-	9.35E+00	8.98E+00	8.38E+00
12	-	9.35E+00	8.99E+00	8.38E+00
13	-	9.35E+00	8.99E+00	8.38E+00
14	-	9.35E+00	8.99E+00	8.38E+00
15	-	9.35E+00	8.99E+00	8.38E+00
16	-	9.35E+00	9.00E+00	8.38E+00
17	-	9.35E+00	9.01E+00	8.39E+00
18	-	9.35E+00	9.03E+00	8.39E+00
19	-	9.36E+00	9.04E+00	8.39E+00
20	-	9.36E+00	9.04E+00	8.39E+00

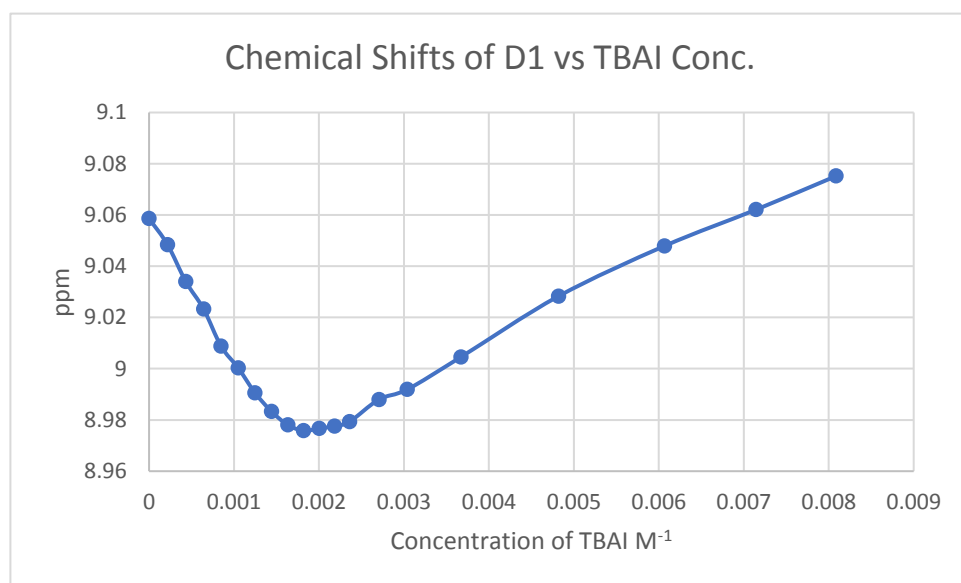
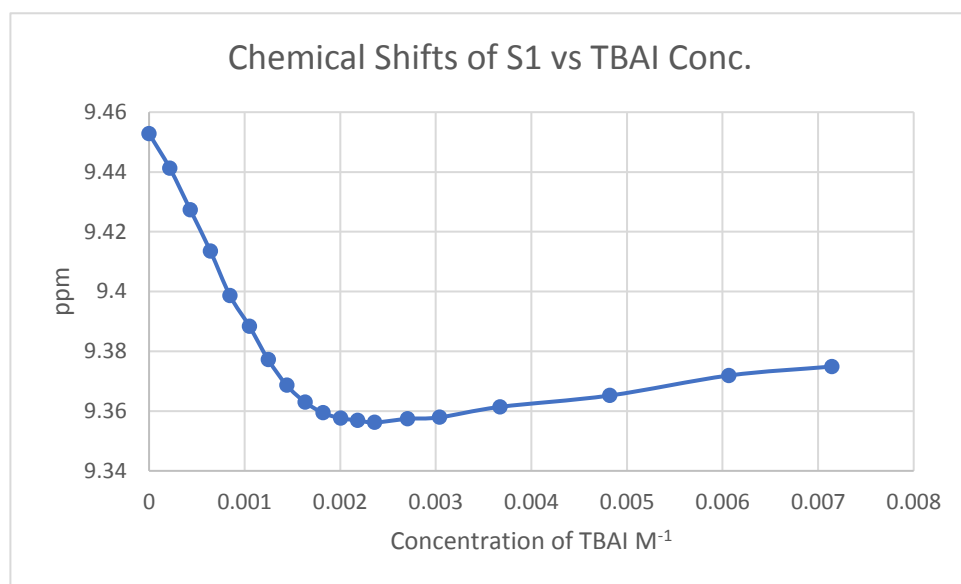
Calculated chemical shifts

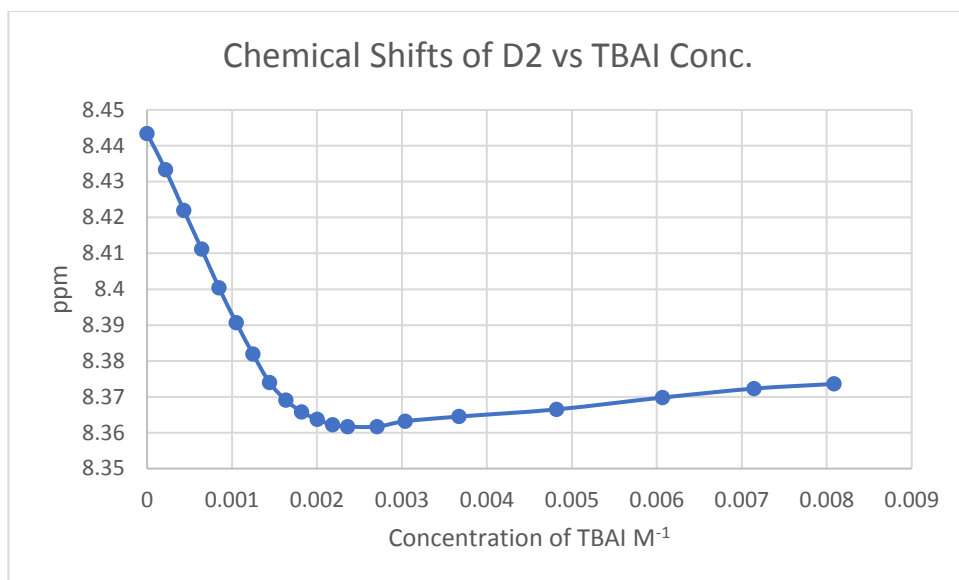
Point	pH	S1	D1	D2
1	-	9.46E+00	9.06E+00	8.44E+00
2	-	9.44E+00	9.05E+00	8.44E+00
3	-	9.42E+00	9.04E+00	8.43E+00
4	-	9.41E+00	9.03E+00	8.42E+00
5	-	9.39E+00	9.01E+00	8.41E+00
6	-	9.38E+00	9.01E+00	8.40E+00
7	-	9.37E+00	9.00E+00	8.39E+00
8	-	9.36E+00	8.99E+00	8.39E+00
9	-	9.35E+00	8.99E+00	8.38E+00
10	-	9.35E+00	8.99E+00	8.38E+00
11	-	9.35E+00	8.99E+00	8.38E+00
12	-	9.35E+00	8.99E+00	8.38E+00
13	-	9.35E+00	8.99E+00	8.38E+00
14	-	9.35E+00	8.99E+00	8.38E+00

15	-	9.35E+00	8.99E+00	8.38E+00
16	-	9.35E+00	9.00E+00	8.38E+00
17	-	9.35E+00	9.01E+00	8.39E+00
18	-	9.36E+00	9.03E+00	8.39E+00
19	-	9.36E+00	9.03E+00	8.39E+00
20	-	9.36E+00	9.04E+00	8.39E+00

Chemical shifts for each nucleus

species	S1	D1	D2
H	9.46E+00	9.06E+00	8.44E+00
GH	9.34E+00	8.97E+00	8.37E+00
G ₂ H	9.42E+00	9.21E+00	8.44E+00





G2XB and TBA⁺I⁻ (Experiment 2)

Species	Log beta	G	H	std. dev.
				0.0957
1	4.6068	1	1	
				0.0874
2	6.9167	2	1	

Converged in 1 iterations with sigma = 1.432568

Species concentrations/mol dm⁻³

Point	pH	T(TBAI)	T(G2XB)	F(TBAI)	F(G2XB)	species 1	species 2
1	-	0.00E+00	1.53E-03	2.49E-91	1.53E-03	1.54E-89	7.85E-178
2	-	2.44E-04	1.53E-03	4.57E-06	1.29E-03	2.39E-04	2.23E-07
3	-	4.83E-04	1.53E-03	1.09E-05	1.06E-03	4.70E-04	1.05E-06
4	-	7.17E-04	1.53E-03	2.04E-05	8.38E-04	6.91E-04	2.88E-06
5	-	9.47E-04	1.53E-03	3.55E-05	6.27E-04	8.98E-04	6.50E-06
6	-	1.17E-03	1.53E-03	6.17E-05	4.34E-04	1.08E-03	1.36E-05
7	-	1.39E-03	1.53E-03	1.10E-04	2.76E-04	1.23E-03	2.76E-05
8	-	1.61E-03	1.53E-03	1.94E-04	1.67E-04	1.31E-03	5.20E-05
9	-	1.82E-03	1.53E-03	3.13E-04	1.06E-04	1.34E-03	8.55E-05
10	-	2.03E-03	1.53E-03	4.51E-04	7.32E-05	1.34E-03	1.23E-04
11	-	2.24E-03	1.53E-03	6.00E-04	5.43E-05	1.32E-03	1.61E-04
12	-	2.44E-03	1.53E-03	7.52E-04	4.24E-05	1.29E-03	1.98E-04
13	-	2.64E-03	1.53E-03	9.07E-04	3.45E-05	1.26E-03	2.34E-04
14	-	3.02E-03	1.53E-03	1.22E-03	2.45E-05	1.21E-03	3.00E-04
15	-	3.39E-03	1.53E-03	1.52E-03	1.87E-05	1.15E-03	3.59E-04
16	-	3.75E-03	1.53E-03	1.83E-03	1.50E-05	1.10E-03	4.12E-04

17	-	4.10E-03	1.53E-03	2.12E-03	1.23E-05	1.06E-03	4.59E-04
18	-	4.76E-03	1.53E-03	2.70E-03	8.99E-06	9.81E-04	5.41E-04
19	-	6.24E-03	1.53E-03	4.03E-03	5.14E-06	8.37E-04	6.89E-04
20	-	7.75E-03	1.53E-03	5.42E-03	3.31E-06	7.25E-04	8.03E-04

Measured chemical shifts

Point	pH	S1	D1	D2
1	-	9.45E+00	9.06E+00	8.44E+00
2	-	9.43E+00	9.04E+00	8.43E+00
3	-	9.41E+00	9.03E+00	8.42E+00
4	-	9.39E+00	9.01E+00	8.41E+00
5	-	9.38E+00	9.00E+00	8.40E+00
6	-	9.36E+00	8.99E+00	8.39E+00
7	-	9.35E+00	8.98E+00	8.38E+00
8	-	9.35E+00	8.98E+00	8.38E+00
9	-	9.34E+00	8.98E+00	8.38E+00
10	-	9.34E+00	8.98E+00	8.38E+00
11	-	9.34E+00	8.98E+00	8.38E+00
12	-	9.34E+00	8.99E+00	8.38E+00
13	-	9.34E+00	8.99E+00	8.38E+00
14	-	9.34E+00	8.99E+00	8.38E+00
15	-	9.34E+00	9.00E+00	8.38E+00
16	-	9.35E+00	9.00E+00	8.38E+00
17	-	9.35E+00	9.01E+00	8.38E+00
18	-	9.35E+00	9.01E+00	8.38E+00
19	-	9.35E+00	9.03E+00	8.39E+00
20	-	9.36E+00	9.04E+00	8.39E+00

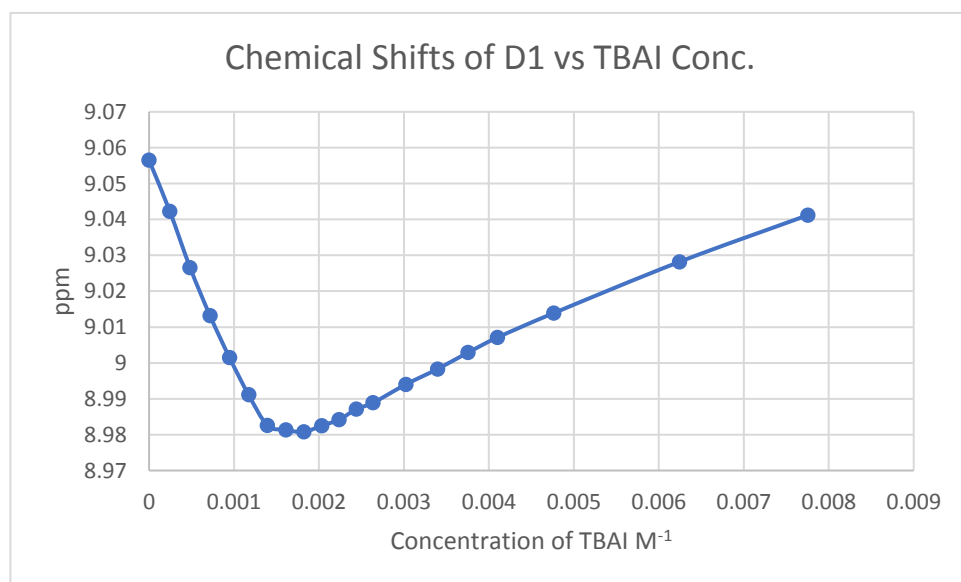
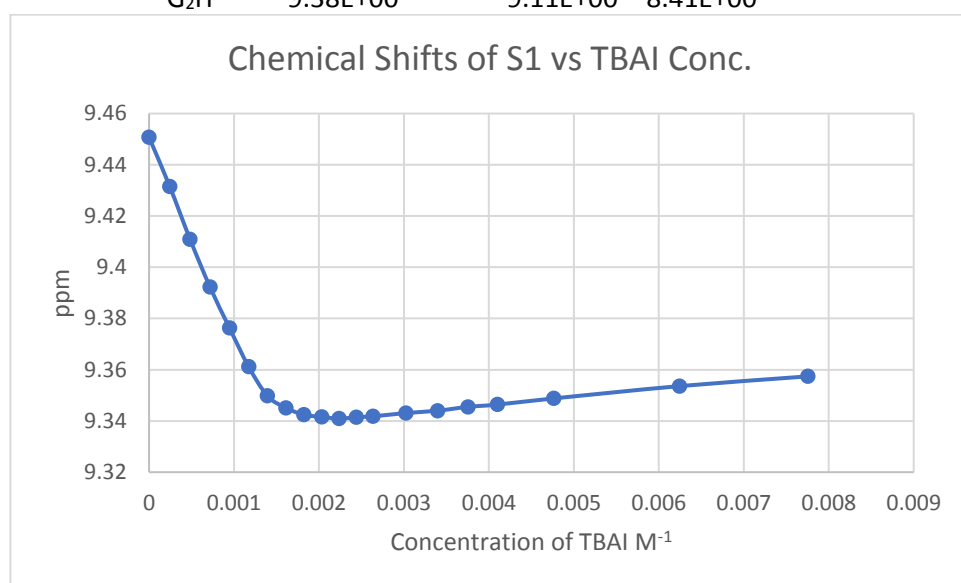
Calculated chemical shifts

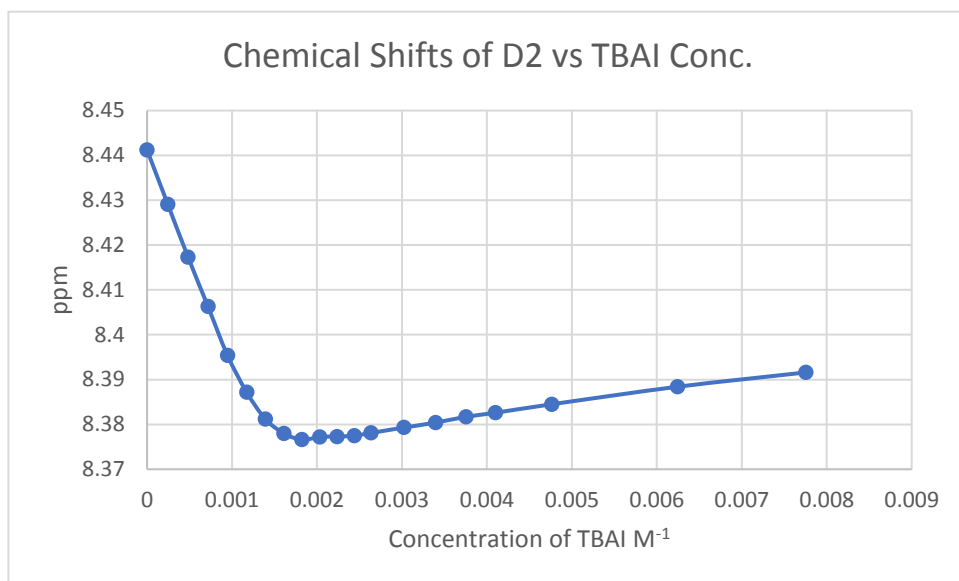
Point	pH	S1	D1	D2
1	-	9.45E+00	9.06E+00	8.44E+00
2	-	9.43E+00	9.04E+00	8.43E+00
3	-	9.41E+00	9.03E+00	8.42E+00
4	-	9.39E+00	9.01E+00	8.41E+00
5	-	9.38E+00	9.00E+00	8.40E+00
6	-	9.36E+00	8.99E+00	8.39E+00
7	-	9.35E+00	8.98E+00	8.38E+00
8	-	9.34E+00	8.98E+00	8.38E+00
9	-	9.34E+00	8.98E+00	8.38E+00
10	-	9.34E+00	8.98E+00	8.38E+00
11	-	9.34E+00	8.98E+00	8.38E+00
12	-	9.34E+00	8.99E+00	8.38E+00
13	-	9.34E+00	8.99E+00	8.38E+00

14	-	9.34E+00	8.99E+00	8.38E+00
15	-	9.34E+00	9.00E+00	8.38E+00
16	-	9.35E+00	9.00E+00	8.38E+00
17	-	9.35E+00	9.01E+00	8.38E+00
18	-	9.35E+00	9.02E+00	8.38E+00
19	-	9.35E+00	9.03E+00	8.39E+00
20	-	9.36E+00	9.04E+00	8.39E+00

Chemical shifts for each nucleus

species	S1	D1	D2
H	9.45E+00	9.06E+00	8.44E+00
GH	9.33E+00	8.97E+00	8.37E+00
G ₂ H	9.38E+00	9.11E+00	8.41E+00





G2XB and TBA⁺I⁻ (Experiment 3)

Species	Log beta	G	H	std. dev.
				0.0599
1	4.6714	1	1	
				0.0581
2	6.767	2	1	

Converged in 1 iterations with sigma = 0.821444

Species concentrations/mol dm⁻³

Point	pH	T(TBAI)	T(G2XB)	F(TBAI)	F(G2XB)	species 1	species 2
1	-	0.00E+00	1.53E-03	2.35E-91	1.53E-03	1.69E-89	4.96E-178
2	-	2.44E-04	1.53E-03	3.95E-06	1.29E-03	2.39E-04	1.18E-07
3	-	4.83E-04	1.53E-03	9.50E-06	1.06E-03	4.72E-04	5.59E-07
4	-	7.17E-04	1.53E-03	1.78E-05	8.34E-04	6.96E-04	1.54E-06
5	-	9.47E-04	1.53E-03	3.13E-05	6.19E-04	9.08E-04	3.54E-06
6	-	1.17E-03	1.53E-03	5.56E-05	4.22E-04	1.10E-03	7.62E-06
7	-	1.39E-03	1.53E-03	1.04E-04	2.58E-04	1.26E-03	1.63E-05
8	-	1.61E-03	1.53E-03	1.94E-04	1.48E-04	1.35E-03	3.27E-05
9	-	1.82E-03	1.53E-03	3.26E-04	9.05E-05	1.38E-03	5.63E-05
10	-	2.03E-03	1.53E-03	4.80E-04	6.16E-05	1.39E-03	8.29E-05
11	-	2.24E-03	1.53E-03	6.42E-04	4.57E-05	1.38E-03	1.10E-04
12	-	2.44E-03	1.53E-03	8.07E-04	3.59E-05	1.36E-03	1.37E-04
13	-	2.64E-03	1.53E-03	9.73E-04	2.93E-05	1.34E-03	1.62E-04
14	-	3.02E-03	1.53E-03	1.30E-03	2.13E-05	1.30E-03	2.11E-04
15	-	3.39E-03	1.53E-03	1.63E-03	1.65E-05	1.26E-03	2.55E-04
16	-	3.75E-03	1.53E-03	1.94E-03	1.34E-05	1.22E-03	2.96E-04
17	-	4.10E-03	1.53E-03	2.25E-03	1.12E-05	1.19E-03	3.33E-04

18	-	4.76E-03	1.53E-03	2.84E-03	8.43E-06	1.12E-03	3.98E-04
19	-	6.24E-03	1.53E-03	4.19E-03	5.09E-06	1.00E-03	5.24E-04
20	-	7.75E-03	1.53E-03	5.60E-03	3.43E-06	9.00E-04	6.28E-04

Measured chemical shifts

Point	pH	S1	D1	D2
1	-	9.45E+00	9.06E+00	8.44E+00
2	-	9.43E+00	9.04E+00	8.43E+00
3	-	9.42E+00	9.03E+00	8.42E+00
4	-	9.40E+00	9.02E+00	8.41E+00
5	-	9.38E+00	9.00E+00	8.40E+00
6	-	9.37E+00	8.99E+00	8.39E+00
7	-	9.35E+00	8.99E+00	8.38E+00
8	-	9.35E+00	8.98E+00	8.38E+00
9	-	9.34E+00	8.98E+00	8.38E+00
10	-	9.34E+00	8.98E+00	8.38E+00
11	-	9.34E+00	8.99E+00	8.38E+00
12	-	9.34E+00	8.99E+00	8.38E+00
13	-	9.34E+00	8.99E+00	8.38E+00
14	-	9.34E+00	8.99E+00	8.38E+00
15	-	9.35E+00	9.00E+00	8.38E+00
16	-	9.35E+00	9.00E+00	8.38E+00
17	-	9.35E+00	9.01E+00	8.38E+00
18	-	9.35E+00	9.01E+00	8.39E+00
19	-	9.35E+00	9.03E+00	8.39E+00
20	-	9.36E+00	9.04E+00	8.39E+00

Calculated chemical shifts

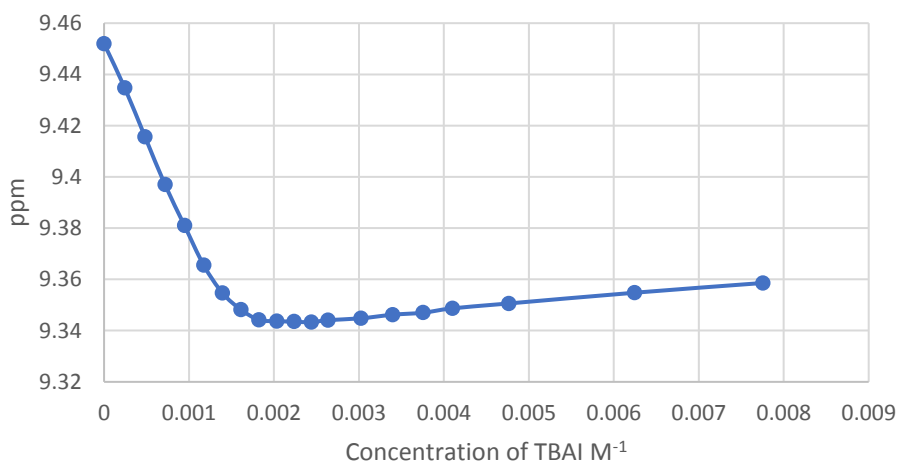
Point	pH	S1	D1	D2
1	-	9.45E+00	9.06E+00	8.44E+00
2	-	9.43E+00	9.04E+00	8.43E+00
3	-	9.42E+00	9.03E+00	8.42E+00
4	-	9.40E+00	9.02E+00	8.41E+00
5	-	9.38E+00	9.01E+00	8.40E+00
6	-	9.37E+00	9.00E+00	8.39E+00
7	-	9.36E+00	8.99E+00	8.38E+00
8	-	9.35E+00	8.98E+00	8.38E+00
9	-	9.34E+00	8.98E+00	8.38E+00
10	-	9.34E+00	8.98E+00	8.38E+00
11	-	9.34E+00	8.98E+00	8.38E+00
12	-	9.34E+00	8.99E+00	8.38E+00
13	-	9.34E+00	8.99E+00	8.38E+00
14	-	9.34E+00	8.99E+00	8.38E+00

15	-	9.35E+00	9.00E+00	8.38E+00
16	-	9.35E+00	9.00E+00	8.38E+00
17	-	9.35E+00	9.01E+00	8.38E+00
18	-	9.35E+00	9.01E+00	8.39E+00
19	-	9.36E+00	9.03E+00	8.39E+00
20	-	9.36E+00	9.04E+00	8.39E+00

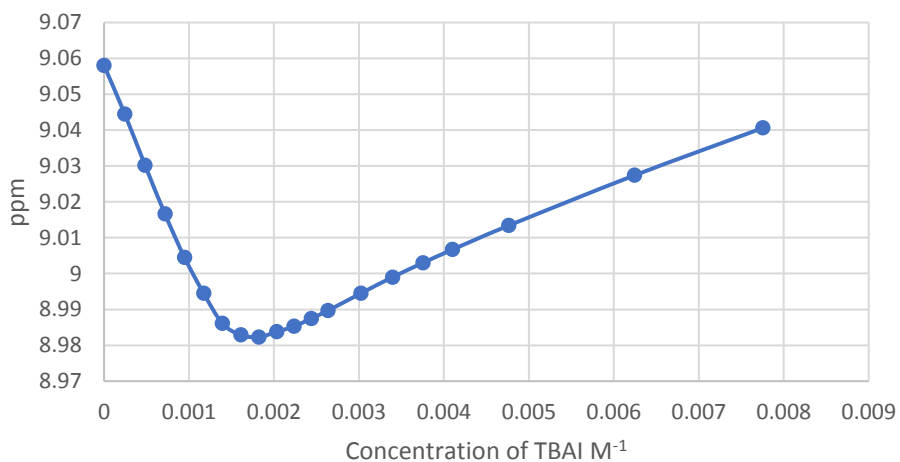
Chemical shifts for each nucleus

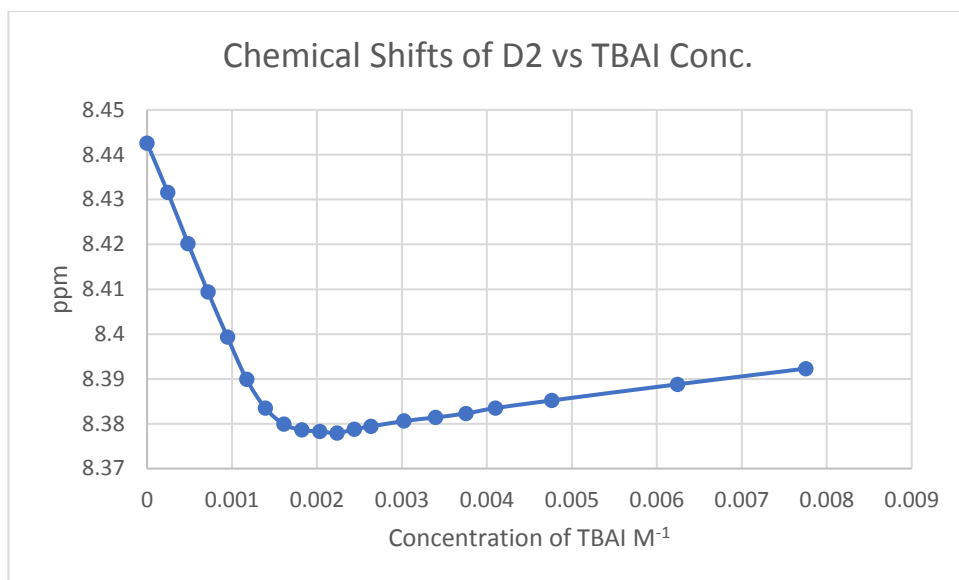
species	S1	D1	D2
H	9.45E+00	9.06E+00	8.44E+00
GH	9.34E+00	8.97E+00	8.37E+00
G ₂ H	9.39E+00	9.14E+00	8.42E+00

Chemical Shifts of S1 vs TBAI Conc.



Chemical Shifts of D1 vs TBAI Conc.





G1XB and TBA⁺Cl⁻ (Experiment 1)

Species	Log beta	G	H	std. dev.
1	3.3312	1	1	0.0515
2	5.2745	2	1	0.1278

Converged in 1 iterations with sigma = 0.146282

Species concentrations/mol dm⁻³

Point	pH	T(TBACl)	T(G1XB)	F(TBACl)	F(G1XB)	species 1	species 2
1	-	0.00E+00	1.63E-03	1.14E-90	1.63E-03	3.96E-90	3.94E-178
2	-	2.11E-04	1.63E-03	5.05E-05	1.47E-03	1.59E-04	7.05E-07
3	-	4.18E-04	1.63E-03	1.08E-04	1.32E-03	3.04E-04	2.87E-06
4	-	6.20E-04	1.63E-03	1.72E-04	1.18E-03	4.36E-04	6.56E-06
5	-	8.19E-04	1.63E-03	2.43E-04	1.06E-03	5.53E-04	1.18E-05
6	-	1.01E-03	1.63E-03	3.21E-04	9.52E-04	6.56E-04	1.85E-05
7	-	1.21E-03	1.63E-03	4.07E-04	8.54E-04	7.45E-04	2.66E-05
8	-	1.39E-03	1.63E-03	4.99E-04	7.68E-04	8.22E-04	3.60E-05
9	-	1.58E-03	1.63E-03	5.97E-04	6.92E-04	8.87E-04	4.65E-05
10	-	1.76E-03	1.63E-03	7.01E-04	6.27E-04	9.42E-04	5.79E-05
11	-	1.94E-03	1.63E-03	8.09E-04	5.69E-04	9.87E-04	7.01E-05
12	-	2.11E-03	1.63E-03	9.21E-04	5.19E-04	1.02E-03	8.28E-05
13	-	2.28E-03	1.63E-03	1.04E-03	4.75E-04	1.05E-03	9.58E-05
14	-	2.62E-03	1.63E-03	1.27E-03	4.04E-04	1.10E-03	1.23E-04
15	-	2.94E-03	1.63E-03	1.51E-03	3.48E-04	1.13E-03	1.50E-04
16	-	3.55E-03	1.63E-03	1.99E-03	2.70E-04	1.15E-03	2.02E-04
17	-	4.66E-03	1.63E-03	2.92E-03	1.83E-04	1.15E-03	2.94E-04

18	-	5.86E-03	1.63E-03	3.98E-03	1.30E-04	1.11E-03	3.87E-04
19	-	6.91E-03	1.63E-03	4.92E-03	1.01E-04	1.07E-03	4.60E-04
20	-	7.82E-03	1.63E-03	5.76E-03	8.31E-05	1.03E-03	5.18E-04

Measured chemical shifts

Point	pH	S1	D1	S2
1	-	9.47E+00	9.08E+00	8.45E+00
2	-	9.47E+00	9.07E+00	8.47E+00
3	-	9.46E+00	9.07E+00	8.49E+00
4	-	9.46E+00	9.07E+00	8.52E+00
5	-	9.45E+00	9.06E+00	8.54E+00
6	-	9.45E+00	9.06E+00	8.56E+00
7	-	9.44E+00	9.06E+00	8.57E+00
8	-	9.44E+00	9.06E+00	8.59E+00
9	-	9.44E+00	9.06E+00	8.60E+00
10	-	9.43E+00	9.06E+00	8.61E+00
11	-	9.43E+00	9.06E+00	8.62E+00
12	-	9.43E+00	9.06E+00	8.63E+00
13	-	9.43E+00	9.06E+00	8.64E+00
14	-	9.43E+00	9.06E+00	8.65E+00
15	-	9.43E+00	9.07E+00	8.66E+00
16	-	9.43E+00	9.07E+00	8.67E+00
17	-	9.43E+00	9.09E+00	8.68E+00
18	-	9.43E+00	9.11E+00	8.68E+00
19	-	9.44E+00	9.12E+00	8.68E+00
20	-	9.44E+00	9.13E+00	8.69E+00

Calculated chemical shifts

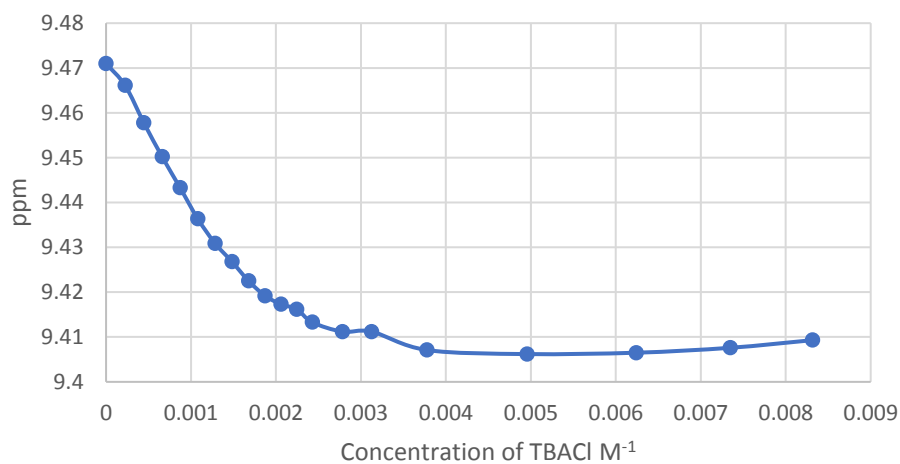
Point	pH	S1	D1	S2
1	-	9.47E+00	9.08E+00	8.45E+00
2	-	9.47E+00	9.07E+00	8.47E+00
3	-	9.46E+00	9.07E+00	8.50E+00
4	-	9.45E+00	9.07E+00	8.52E+00
5	-	9.45E+00	9.06E+00	8.54E+00
6	-	9.45E+00	9.06E+00	8.56E+00
7	-	9.44E+00	9.06E+00	8.57E+00
8	-	9.44E+00	9.06E+00	8.59E+00
9	-	9.44E+00	9.06E+00	8.60E+00
10	-	9.43E+00	9.06E+00	8.61E+00
11	-	9.43E+00	9.06E+00	8.62E+00
12	-	9.43E+00	9.06E+00	8.63E+00
13	-	9.43E+00	9.06E+00	8.63E+00
14	-	9.43E+00	9.06E+00	8.65E+00

15	-	9.43E+00	9.07E+00	8.65E+00
16	-	9.43E+00	9.07E+00	8.67E+00
17	-	9.43E+00	9.09E+00	8.68E+00
18	-	9.43E+00	9.11E+00	8.68E+00
19	-	9.44E+00	9.12E+00	8.69E+00
20	-	9.44E+00	9.13E+00	8.69E+00

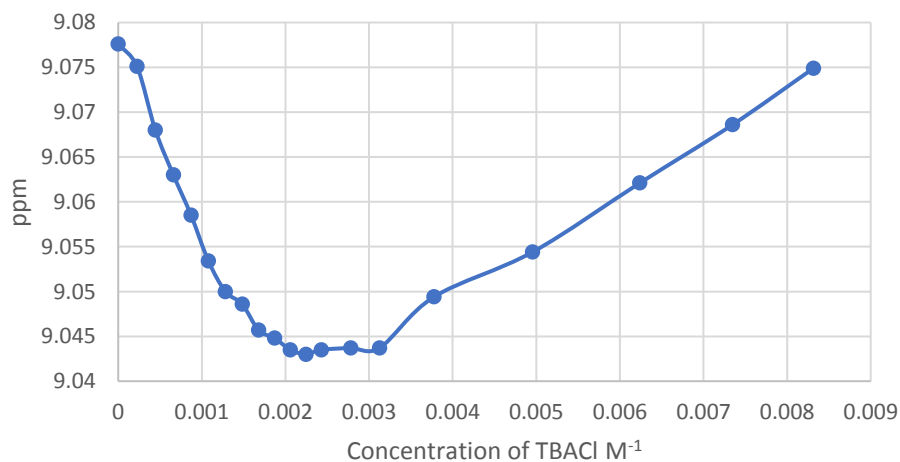
Chemical shifts for each nucleus

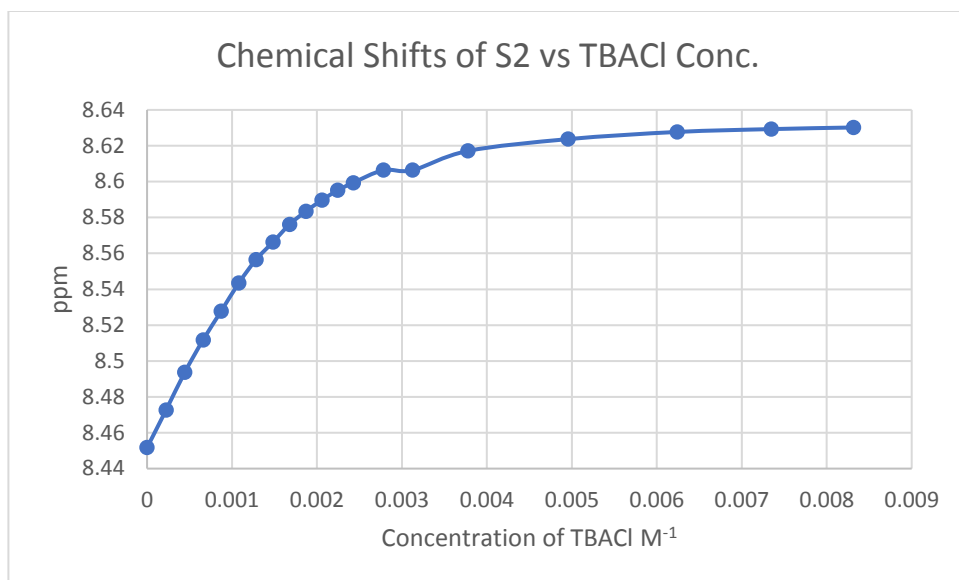
species	S1	D1	S2
H	9.47E+00	9.08E+00	8.45E+00
GH	9.40E+00	9.02E+00	8.72E+00
G ₂ H	9.50E+00	9.35E+00	8.66E+00

Chemical Shifts of S1 vs TBACl Conc.



Chemical Shifts of D1 vs TBACl Conc.





G1XB and TBA⁺Cl⁻ (Experiment 2)

Species	Log beta	G	H	std. dev.
				0.0369
1	3.4291	1	1	
				0.0963
2	5.367	2	1	

Converged in 1 iterations with sigma = 1.247361

Species concentrations/mol dm⁻³

Point	pH	T(TBACl)	T(G1XB)	F(TBACl)	F(G1XB)	species 1	species 2
1	-	0.00E+00	1.50E-03	9.71E-91	1.50E-03	3.92E-90	3.30E-178
2	-	2.38E-04	1.50E-03	5.19E-05	1.32E-03	1.84E-04	8.28E-07
3	-	4.70E-04	1.50E-03	1.13E-04	1.15E-03	3.50E-04	3.44E-06
4	-	6.99E-04	1.50E-03	1.86E-04	9.98E-04	4.97E-04	7.99E-06
5	-	9.23E-04	1.50E-03	2.69E-04	8.64E-04	6.24E-04	1.46E-05
6	-	1.14E-03	1.50E-03	3.64E-04	7.48E-04	7.32E-04	2.31E-05
7	-	1.36E-03	1.50E-03	4.71E-04	6.49E-04	8.20E-04	3.35E-05
8	-	1.57E-03	1.50E-03	5.87E-04	5.66E-04	8.92E-04	4.54E-05
9	-	1.78E-03	1.50E-03	7.12E-04	4.96E-04	9.48E-04	5.85E-05
10	-	1.98E-03	1.50E-03	8.43E-04	4.38E-04	9.92E-04	7.25E-05
11	-	2.18E-03	1.50E-03	9.80E-04	3.90E-04	1.03E-03	8.72E-05
12	-	2.38E-03	1.50E-03	1.12E-03	3.49E-04	1.05E-03	1.02E-04
13	-	2.57E-03	1.50E-03	1.26E-03	3.15E-04	1.07E-03	1.17E-04
14	-	2.95E-03	1.50E-03	1.56E-03	2.62E-04	1.09E-03	1.48E-04
15	-	3.31E-03	1.50E-03	1.85E-03	2.22E-04	1.10E-03	1.77E-04
16	-	3.66E-03	1.50E-03	2.14E-03	1.92E-04	1.11E-03	2.05E-04
17	-	4.00E-03	1.50E-03	2.43E-03	1.69E-04	1.10E-03	2.32E-04

18	-	4.64E-03	1.50E-03	2.99E-03	1.35E-04	1.09E-03	2.82E-04
19	-	6.09E-03	1.50E-03	4.29E-03	8.94E-05	1.03E-03	3.83E-04
20	-	7.56E-03	1.50E-03	5.65E-03	6.37E-05	9.66E-04	4.73E-04

Measured chemical shifts

Point	pH	S1	D1	S2
1	-	9.47E+00	9.08E+00	8.45E+00
2	-	9.46E+00	9.07E+00	8.48E+00
3	-	9.46E+00	9.07E+00	8.51E+00
4	-	9.45E+00	9.06E+00	8.53E+00
5	-	9.44E+00	9.06E+00	8.56E+00
6	-	9.44E+00	9.06E+00	8.58E+00
7	-	9.44E+00	9.06E+00	8.59E+00
8	-	9.43E+00	9.06E+00	8.61E+00
9	-	9.43E+00	9.06E+00	8.62E+00
10	-	9.43E+00	9.06E+00	8.63E+00
11	-	9.43E+00	9.06E+00	8.64E+00
12	-	9.43E+00	9.06E+00	8.65E+00
13	-	9.43E+00	9.06E+00	8.65E+00
14	-	9.43E+00	9.07E+00	8.66E+00
15	-	9.43E+00	9.07E+00	8.67E+00
16	-	9.43E+00	9.08E+00	8.67E+00
17	-	9.43E+00	9.08E+00	8.67E+00
18	-	9.43E+00	9.09E+00	8.68E+00
19	-	9.43E+00	9.11E+00	8.68E+00
20	-	9.44E+00	9.13E+00	8.69E+00

Calculated chemical shifts

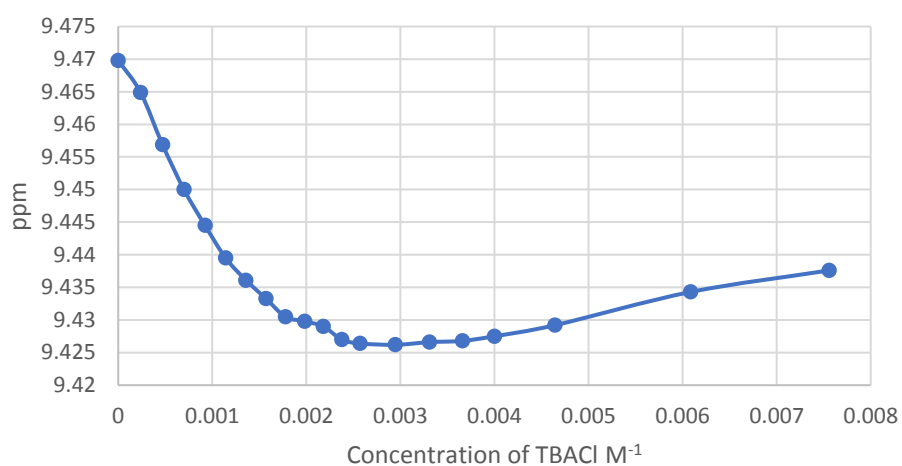
Point	pH	S1	D1	S2
1	-	9.47E+00	9.08E+00	8.45E+00
2	-	9.46E+00	9.07E+00	8.48E+00
3	-	9.46E+00	9.07E+00	8.51E+00
4	-	9.45E+00	9.06E+00	8.53E+00
5	-	9.44E+00	9.06E+00	8.56E+00
6	-	9.44E+00	9.06E+00	8.58E+00
7	-	9.44E+00	9.06E+00	8.59E+00
8	-	9.43E+00	9.06E+00	8.61E+00
9	-	9.43E+00	9.06E+00	8.62E+00
10	-	9.43E+00	9.06E+00	8.63E+00
11	-	9.43E+00	9.06E+00	8.64E+00
12	-	9.43E+00	9.06E+00	8.65E+00
13	-	9.43E+00	9.06E+00	8.65E+00
14	-	9.43E+00	9.07E+00	8.66E+00
15	-	9.43E+00	9.07E+00	8.67E+00

16	-	9.43E+00	9.08E+00	8.67E+00
17	-	9.43E+00	9.08E+00	8.67E+00
18	-	9.43E+00	9.09E+00	8.68E+00
19	-	9.43E+00	9.11E+00	8.68E+00
20	-	9.44E+00	9.13E+00	8.69E+00

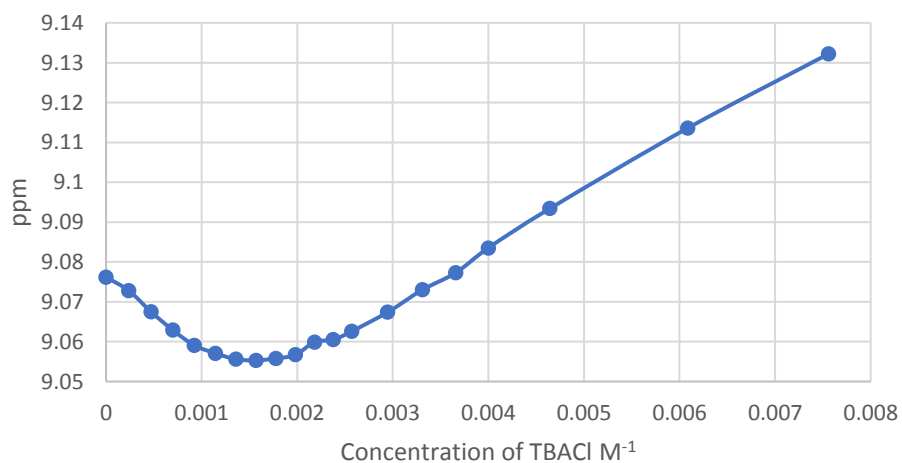
Chemical shifts for each nucleus

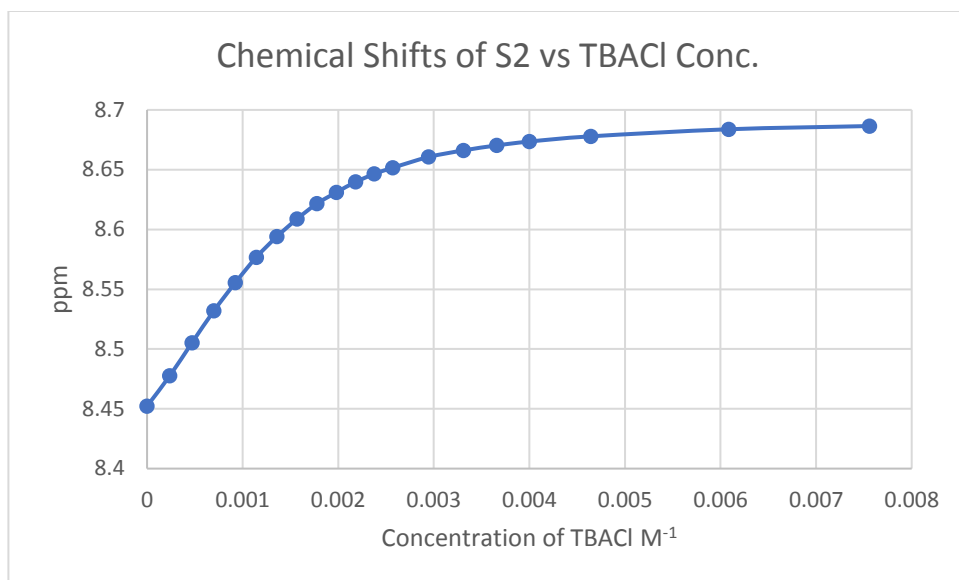
species	S1	D1	S2
H	9.47E+00	9.08E+00	8.45E+00
GH	9.41E+00	9.03E+00	8.71E+00
G ₂ H	9.50E+00	9.36E+00	8.68E+00

Chemical Shifts of S1 vs TBACl Conc.



Chemical Shifts of D1 vs TBACl Conc.





G1XB and TBA⁺Cl⁻ (Experiment 3)

Species	Log beta	G	H	std. dev.
				0.0345
1	3.4991	1	1	
				0.0852
2	5.4517	2	1	

Converged in 1 iterations with sigma = 1.179944

Species concentrations/mol dm⁻³

Point	pH	T(TBACl)	T(G1XB)	F(TBACl)	F(G1XB)	species 1	species 2
1	-	0.00E+00	1.50E-03	8.88E-91	1.50E-03	4.21E-90	3.35E-178
2	-	2.38E-04	1.50E-03	4.59E-05	1.31E-03	1.90E-04	7.82E-07
3	-	4.70E-04	1.50E-03	1.01E-04	1.14E-03	3.63E-04	3.29E-06
4	-	6.99E-04	1.50E-03	1.67E-04	9.79E-04	5.16E-04	7.73E-06
5	-	9.23E-04	1.50E-03	2.45E-04	8.40E-04	6.49E-04	1.43E-05
6	-	1.14E-03	1.50E-03	3.35E-04	7.19E-04	7.61E-04	2.29E-05
7	-	1.36E-03	1.50E-03	4.38E-04	6.17E-04	8.53E-04	3.35E-05
8	-	1.57E-03	1.50E-03	5.52E-04	5.31E-04	9.26E-04	4.58E-05
9	-	1.78E-03	1.50E-03	6.75E-04	4.61E-04	9.83E-04	5.95E-05
10	-	1.98E-03	1.50E-03	8.06E-04	4.03E-04	1.03E-03	7.42E-05
11	-	2.18E-03	1.50E-03	9.44E-04	3.55E-04	1.06E-03	8.95E-05
12	-	2.38E-03	1.50E-03	1.08E-03	3.16E-04	1.08E-03	1.05E-04
13	-	2.57E-03	1.50E-03	1.23E-03	2.83E-04	1.10E-03	1.21E-04
14	-	2.95E-03	1.50E-03	1.52E-03	2.33E-04	1.12E-03	1.53E-04
15	-	3.31E-03	1.50E-03	1.82E-03	1.96E-04	1.12E-03	1.83E-04
16	-	3.66E-03	1.50E-03	2.11E-03	1.68E-04	1.12E-03	2.12E-04
17	-	4.00E-03	1.50E-03	2.40E-03	1.47E-04	1.12E-03	2.40E-04

18	-	4.64E-03	1.50E-03	2.97E-03	1.17E-04	1.09E-03	2.91E-04
19	-	6.09E-03	1.50E-03	4.27E-03	7.66E-05	1.03E-03	3.95E-04
20	-	7.56E-03	1.50E-03	5.62E-03	5.43E-05	9.63E-04	4.86E-04

Measured chemical shifts

Point	pH	S1	D1	S2
1	-	9.47E+00	9.08E+00	8.45E+00
2	-	9.46E+00	9.07E+00	8.48E+00
3	-	9.45E+00	9.07E+00	8.51E+00
4	-	9.45E+00	9.06E+00	8.53E+00
5	-	9.44E+00	9.06E+00	8.56E+00
6	-	9.44E+00	9.06E+00	8.58E+00
7	-	9.43E+00	9.05E+00	8.60E+00
8	-	9.43E+00	9.06E+00	8.61E+00
9	-	9.43E+00	9.06E+00	8.62E+00
10	-	9.43E+00	9.06E+00	8.63E+00
11	-	9.43E+00	9.06E+00	8.64E+00
12	-	9.43E+00	9.06E+00	8.65E+00
13	-	9.43E+00	9.06E+00	8.65E+00
14	-	9.42E+00	9.07E+00	8.66E+00
15	-	9.43E+00	9.07E+00	8.67E+00
16	-	9.43E+00	9.08E+00	8.67E+00
17	-	9.43E+00	9.08E+00	8.67E+00
18	-	9.43E+00	9.10E+00	8.68E+00
19	-	9.43E+00	9.12E+00	8.68E+00
20	-	9.44E+00	9.14E+00	8.69E+00

Calculated chemical shifts

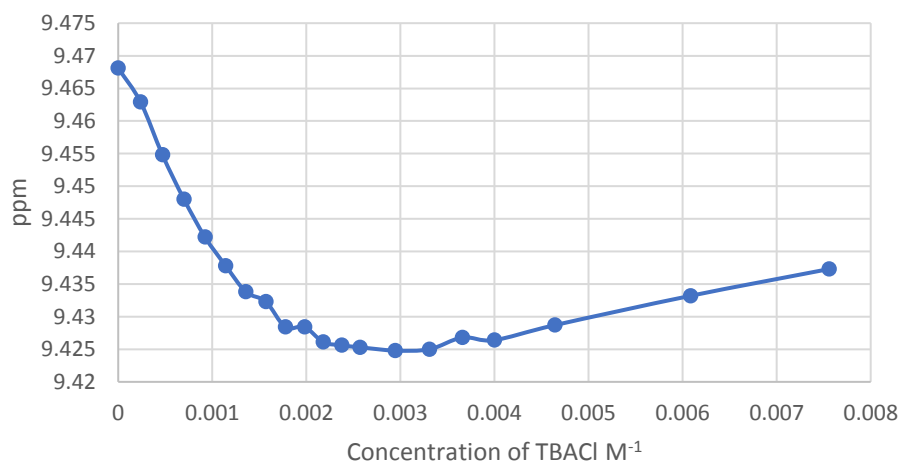
Point	pH	S1	D1	S2
1	-	9.47E+00	9.08E+00	8.45E+00
2	-	9.46E+00	9.07E+00	8.48E+00
3	-	9.45E+00	9.07E+00	8.51E+00
4	-	9.45E+00	9.06E+00	8.54E+00
5	-	9.44E+00	9.06E+00	8.56E+00
6	-	9.44E+00	9.06E+00	8.58E+00
7	-	9.43E+00	9.06E+00	8.60E+00
8	-	9.43E+00	9.06E+00	8.61E+00
9	-	9.43E+00	9.06E+00	8.62E+00
10	-	9.43E+00	9.06E+00	8.63E+00
11	-	9.43E+00	9.06E+00	8.64E+00
12	-	9.43E+00	9.06E+00	8.65E+00
13	-	9.43E+00	9.06E+00	8.65E+00
14	-	9.43E+00	9.07E+00	8.66E+00
15	-	9.43E+00	9.07E+00	8.67E+00

16	-	9.43E+00	9.08E+00	8.67E+00
17	-	9.43E+00	9.09E+00	8.67E+00
18	-	9.43E+00	9.10E+00	8.68E+00
19	-	9.43E+00	9.12E+00	8.68E+00
20	-	9.44E+00	9.14E+00	8.69E+00

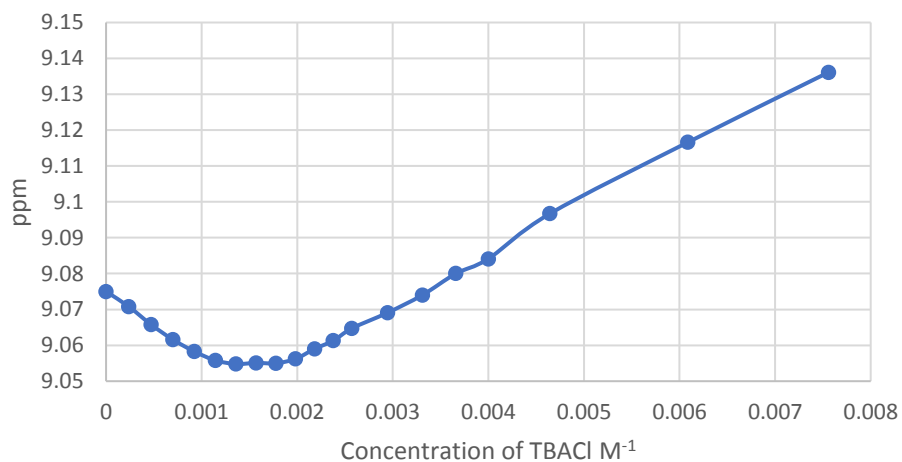
Chemical shifts for each nucleus

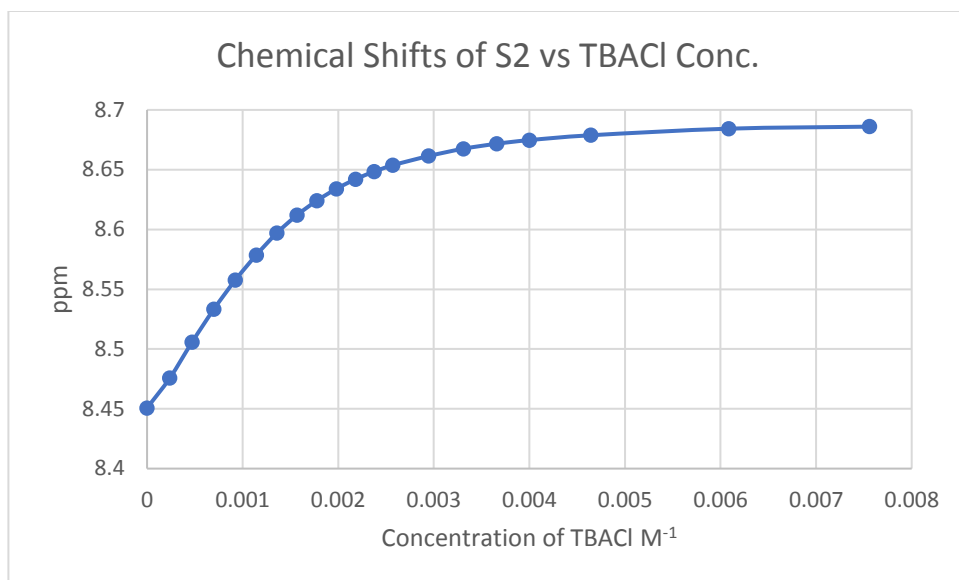
species	S1	D1	S2
H	9.47E+00	9.08E+00	8.45E+00
GH	9.41E+00	9.03E+00	8.70E+00
G ₂ H	9.50E+00	9.36E+00	8.68E+00

Chemical Shifts of S1 vs TBACl Conc.



Chemical Shifts of D1 vs TBACl Conc.





G1XB and TBA⁺Br⁻ (Experiment 1)

Species	Log beta	G	H	std. dev.
				0.0894
1	3.5325	1	1	
				0.2984
2	5.2916	2	1	

Converged in 1 iterations with sigma = 0.238149

Species concentrations/mol dm⁻³

Point	pH	T(TBABr)	T(G1XB)	F(TBABr)	F(G1XB)	species 1	species 2
1	-	0.00E+00	1.65E-03	8.90E-91	1.65E-03	5.01E-90	2.56E-178
2	-	1.70E-04	1.65E-03	2.75E-05	1.51E-03	1.42E-04	2.24E-07
3	-	3.36E-04	1.65E-03	5.88E-05	1.37E-03	2.75E-04	9.29E-07
4	-	4.99E-04	1.65E-03	9.41E-05	1.25E-03	4.00E-04	2.17E-06
5	-	6.59E-04	1.65E-03	1.34E-04	1.13E-03	5.17E-04	3.98E-06
6	-	8.16E-04	1.65E-03	1.79E-04	1.02E-03	6.24E-04	6.42E-06
7	-	9.70E-04	1.65E-03	2.30E-04	9.21E-04	7.21E-04	9.51E-06
8	-	1.12E-03	1.65E-03	2.86E-04	8.29E-04	8.08E-04	1.33E-05
9	-	1.27E-03	1.65E-03	3.48E-04	7.47E-04	8.86E-04	1.77E-05
10	-	1.41E-03	1.65E-03	4.15E-04	6.74E-04	9.54E-04	2.27E-05
11	-	1.56E-03	1.65E-03	4.88E-04	6.10E-04	1.01E-03	2.84E-05
12	-	1.70E-03	1.65E-03	5.65E-04	5.53E-04	1.06E-03	3.45E-05
13	-	1.84E-03	1.65E-03	6.46E-04	5.03E-04	1.11E-03	4.11E-05
14	-	2.10E-03	1.65E-03	8.19E-04	4.21E-04	1.17E-03	5.52E-05
15	-	2.36E-03	1.65E-03	1.00E-03	3.59E-04	1.22E-03	7.02E-05
16	-	2.86E-03	1.65E-03	1.38E-03	2.72E-04	1.28E-03	1.01E-04
17	-	3.32E-03	1.65E-03	1.75E-03	2.18E-04	1.30E-03	1.31E-04

18	-	5.23E-03	1.65E-03	3.44E-03	1.10E-04	1.29E-03	2.54E-04
19	-	6.69E-03	1.65E-03	4.77E-03	7.60E-05	1.24E-03	3.39E-04
20	-	8.30E-03	1.65E-03	6.28E-03	5.48E-05	1.17E-03	4.23E-04

Measured chemical shifts

Point	pH	S1	D1	S2
1	-	9.47E+00	9.08E+00	8.45E+00
2	-	9.47E+00	9.07E+00	8.47E+00
3	-	9.46E+00	9.07E+00	8.49E+00
4	-	9.45E+00	9.07E+00	8.50E+00
5	-	9.45E+00	9.06E+00	8.54E+00
6	-	9.44E+00	9.06E+00	8.54E+00
7	-	9.44E+00	9.06E+00	8.55E+00
8	-	9.44E+00	9.05E+00	8.56E+00
9	-	9.43E+00	9.05E+00	8.57E+00
10	-	9.43E+00	9.05E+00	8.58E+00
11	-	9.43E+00	9.05E+00	8.59E+00
12	-	9.43E+00	9.05E+00	8.60E+00
13	-	9.42E+00	9.05E+00	8.60E+00
14	-	9.42E+00	9.05E+00	8.62E+00
15	-	9.42E+00	9.05E+00	8.62E+00
16	-	9.42E+00	9.05E+00	8.64E+00
17	-	9.42E+00	9.06E+00	8.64E+00
18	-	9.42E+00	9.08E+00	8.66E+00
19	-	9.42E+00	9.09E+00	8.66E+00
20	-	9.42E+00	9.11E+00	8.66E+00

Calculated chemical shifts

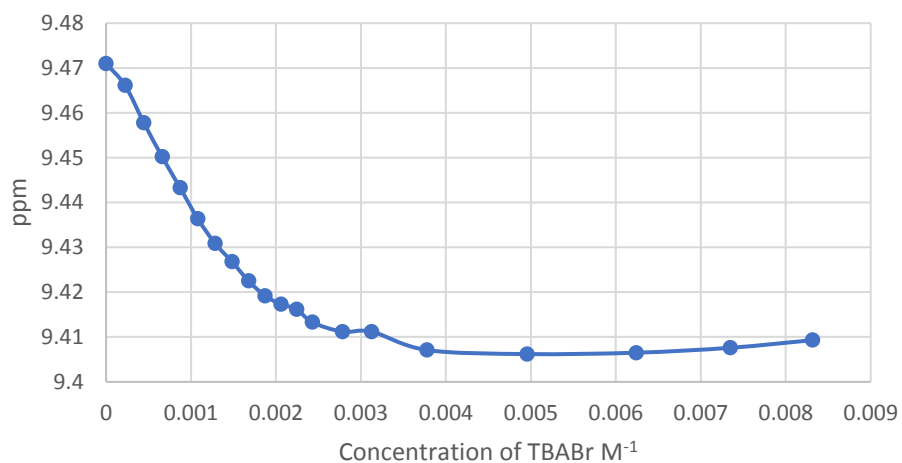
Point	pH	S1	D1	S2
1	-	9.47E+00	9.08E+00	8.45E+00
2	-	9.47E+00	9.07E+00	8.47E+00
3	-	9.46E+00	9.07E+00	8.49E+00
4	-	9.45E+00	9.07E+00	8.51E+00
5	-	9.45E+00	9.06E+00	8.52E+00
6	-	9.44E+00	9.06E+00	8.54E+00
7	-	9.44E+00	9.06E+00	8.55E+00
8	-	9.44E+00	9.05E+00	8.56E+00
9	-	9.43E+00	9.05E+00	8.57E+00
10	-	9.43E+00	9.05E+00	8.58E+00
11	-	9.43E+00	9.05E+00	8.59E+00
12	-	9.43E+00	9.05E+00	8.60E+00
13	-	9.42E+00	9.05E+00	8.61E+00
14	-	9.42E+00	9.05E+00	8.62E+00
15	-	9.42E+00	9.05E+00	8.62E+00

16	-	9.42E+00	9.05E+00	8.64E+00
17	-	9.42E+00	9.06E+00	8.64E+00
18	-	9.42E+00	9.08E+00	8.66E+00
19	-	9.42E+00	9.09E+00	8.66E+00
20	-	9.42E+00	9.11E+00	8.66E+00

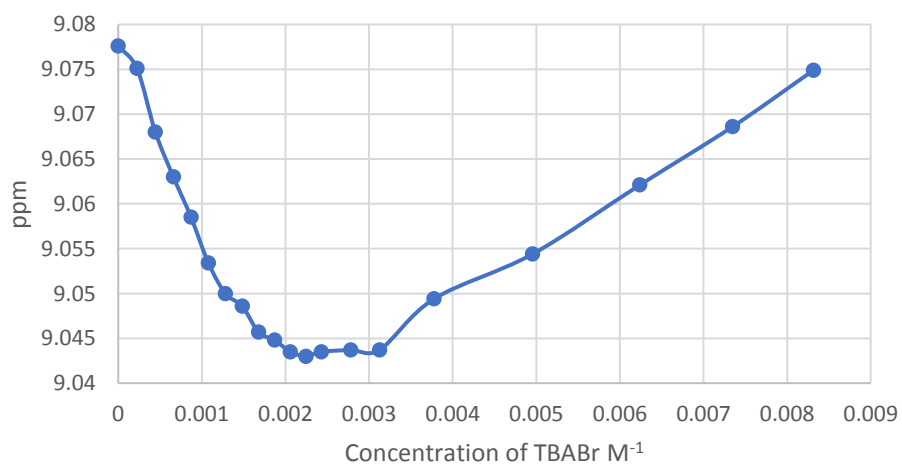
Chemical shifts for each nucleus

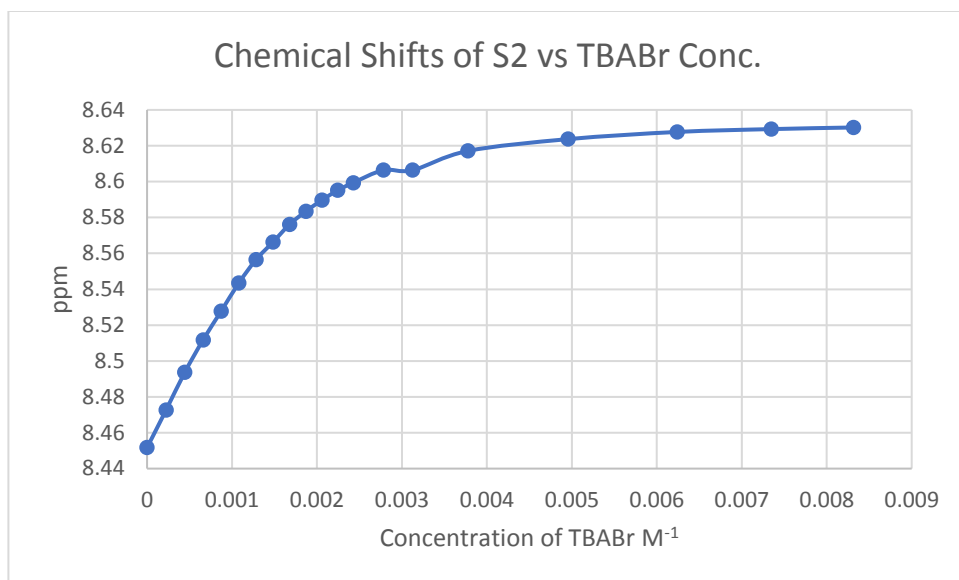
species	S1	D1	S2
H	9.47E+00	9.08E+00	8.45E+00
GH	9.40E+00	9.02E+00	8.67E+00
G ₂ H	9.48E+00	9.34E+00	8.66E+00

Chemical Shifts of S1 vs TBABr Conc.



Chemical Shifts of D1 vs TBABr Conc.





G1XB and TBA⁺Br⁻ (Experiment 2)

Species	Log beta	G	H	std. dev.
				0.0169
1	3.7139	1	1	
				0.0433
2	5.7136	2	1	

Converged in 1 iterations with sigma = 0.054476

Species concentrations/mol dm⁻³

Point	pH	T(TBABr)	T(G1XB)	F(TBABr)	F(G1XB)	species 1	species 2
1	-	0.00E+00	1.50E-03	6.59E-91	1.50E-03	5.12E-90	3.37E-178
2	-	2.42E-04	1.50E-03	3.13E-05	1.29E-03	2.09E-04	6.55E-07
3	-	4.79E-04	1.50E-03	7.09E-05	1.10E-03	4.03E-04	2.85E-06
4	-	7.12E-04	1.50E-03	1.21E-04	9.19E-04	5.77E-04	6.98E-06
5	-	9.40E-04	1.50E-03	1.85E-04	7.61E-04	7.28E-04	1.34E-05
6	-	1.16E-03	1.50E-03	2.64E-04	6.26E-04	8.55E-04	2.25E-05
7	-	1.38E-03	1.50E-03	3.60E-04	5.13E-04	9.55E-04	3.43E-05
8	-	1.60E-03	1.50E-03	4.71E-04	4.23E-04	1.03E-03	4.85E-05
9	-	1.81E-03	1.50E-03	5.95E-04	3.52E-04	1.09E-03	6.46E-05
10	-	2.02E-03	1.50E-03	7.30E-04	2.97E-04	1.12E-03	8.20E-05
11	-	2.22E-03	1.50E-03	8.73E-04	2.54E-04	1.15E-03	1.00E-04
12	-	2.42E-03	1.50E-03	1.02E-03	2.20E-04	1.16E-03	1.19E-04
13	-	2.62E-03	1.50E-03	1.17E-03	1.93E-04	1.17E-03	1.37E-04
14	-	3.00E-03	1.50E-03	1.48E-03	1.54E-04	1.18E-03	1.74E-04
15	-	3.37E-03	1.50E-03	1.79E-03	1.26E-04	1.17E-03	2.08E-04
16	-	3.73E-03	1.50E-03	2.09E-03	1.07E-04	1.16E-03	2.41E-04
17	-	4.07E-03	1.50E-03	2.39E-03	9.21E-05	1.14E-03	2.72E-04

18	-	4.73E-03	1.50E-03	2.97E-03	7.18E-05	1.10E-03	3.28E-04
19	-	6.20E-03	1.50E-03	4.31E-03	4.57E-05	1.02E-03	4.38E-04
20	-	7.70E-03	1.50E-03	5.70E-03	3.18E-05	9.38E-04	5.34E-04

Measured chemical shifts

Point	pH	S1	D1	S2	D3	D4
1	-	9.47E+00	9.08E+00	8.45E+00	8.43E+00	8.31E+00
2	-	9.46E+00	9.07E+00	8.48E+00	8.42E+00	8.30E+00
3	-	9.45E+00	9.06E+00	8.51E+00	8.42E+00	8.29E+00
4	-	9.44E+00	9.06E+00	8.54E+00	8.41E+00	8.28E+00
5	-	9.44E+00	9.05E+00	8.56E+00	8.41E+00	8.28E+00
6	-	9.43E+00	9.05E+00	8.58E+00	8.41E+00	8.27E+00
7	-	9.43E+00	9.05E+00	8.59E+00	8.41E+00	8.27E+00
8	-	9.42E+00	9.05E+00	8.61E+00	8.40E+00	8.26E+00
9	-	9.42E+00	9.05E+00	8.61E+00	8.40E+00	8.26E+00
10	-	9.42E+00	9.05E+00	8.62E+00	8.40E+00	8.26E+00
11	-	9.42E+00	9.05E+00	8.63E+00	8.40E+00	8.26E+00
12	-	9.42E+00	9.05E+00	8.63E+00	8.40E+00	8.25E+00
13	-	9.42E+00	9.05E+00	8.64E+00	8.40E+00	8.25E+00
14	-	9.42E+00	9.06E+00	8.64E+00	8.40E+00	8.25E+00
15	-	9.42E+00	9.06E+00	8.65E+00	8.40E+00	8.25E+00
16	-	9.42E+00	9.07E+00	8.65E+00	8.40E+00	8.25E+00
17	-	9.42E+00	9.07E+00	8.65E+00	8.40E+00	8.25E+00
18	-	9.42E+00	9.08E+00	8.66E+00	8.40E+00	8.25E+00
19	-	9.42E+00	9.09E+00	8.66E+00	8.40E+00	8.24E+00
20	-	9.42E+00	9.11E+00	8.66E+00	8.41E+00	8.24E+00

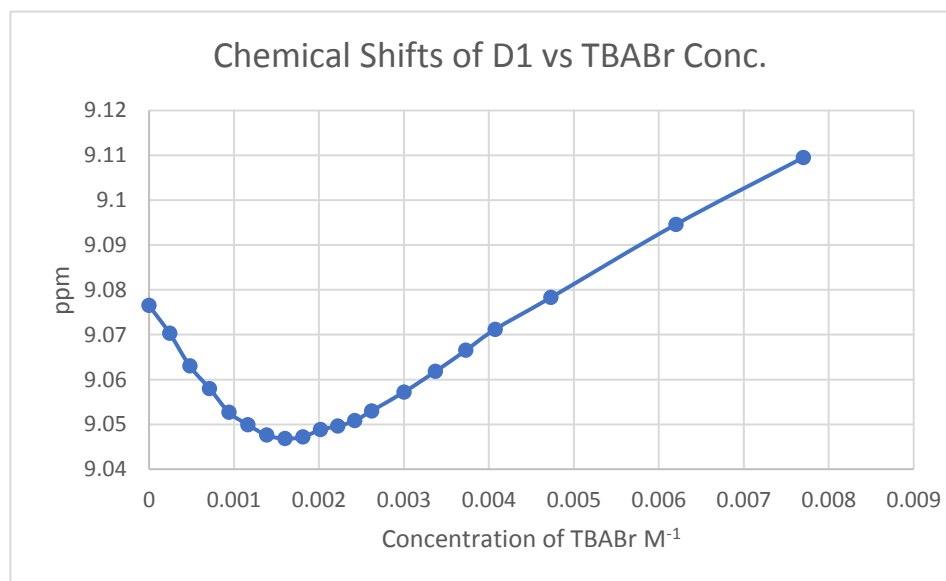
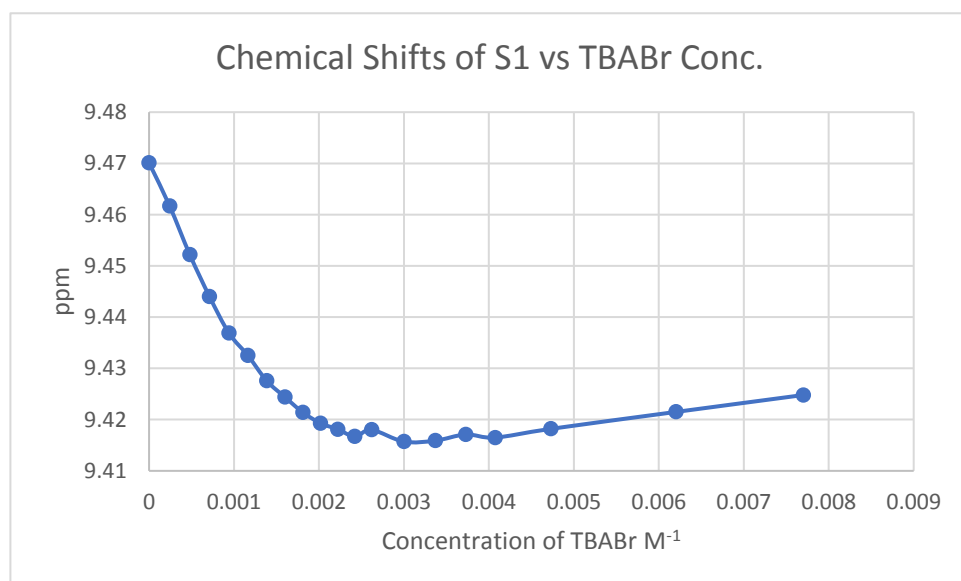
Calculated chemical shifts

Point	pH	S1	D1	S2	D3	D4
1	-	9.47E+00	9.08E+00	8.45E+00	8.43E+00	8.31E+00
2	-	9.46E+00	9.07E+00	8.48E+00	8.42E+00	8.30E+00
3	-	9.45E+00	9.06E+00	8.51E+00	8.42E+00	8.29E+00
4	-	9.44E+00	9.06E+00	8.54E+00	8.41E+00	8.28E+00
5	-	9.44E+00	9.05E+00	8.56E+00	8.41E+00	8.28E+00
6	-	9.43E+00	9.05E+00	8.58E+00	8.41E+00	8.27E+00
7	-	9.43E+00	9.05E+00	8.59E+00	8.41E+00	8.27E+00
8	-	9.42E+00	9.05E+00	8.61E+00	8.40E+00	8.26E+00
9	-	9.42E+00	9.05E+00	8.62E+00	8.40E+00	8.26E+00
10	-	9.42E+00	9.05E+00	8.62E+00	8.40E+00	8.26E+00
11	-	9.42E+00	9.05E+00	8.63E+00	8.40E+00	8.25E+00
12	-	9.42E+00	9.05E+00	8.63E+00	8.40E+00	8.25E+00
13	-	9.42E+00	9.05E+00	8.64E+00	8.40E+00	8.25E+00
14	-	9.42E+00	9.06E+00	8.64E+00	8.40E+00	8.25E+00
15	-	9.42E+00	9.06E+00	8.65E+00	8.40E+00	8.25E+00

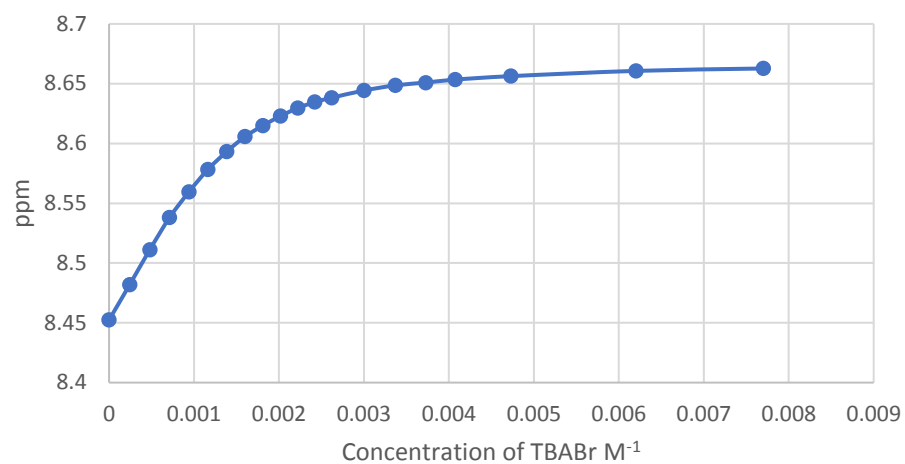
16	-	9.42E+00	9.07E+00	8.65E+00	8.40E+00	8.25E+00
17	-	9.42E+00	9.07E+00	8.65E+00	8.40E+00	8.25E+00
18	-	9.42E+00	9.08E+00	8.66E+00	8.40E+00	8.25E+00
19	-	9.42E+00	9.10E+00	8.66E+00	8.40E+00	8.24E+00
20	-	9.42E+00	9.11E+00	8.66E+00	8.41E+00	8.24E+00

Chemical shifts for each nucleus

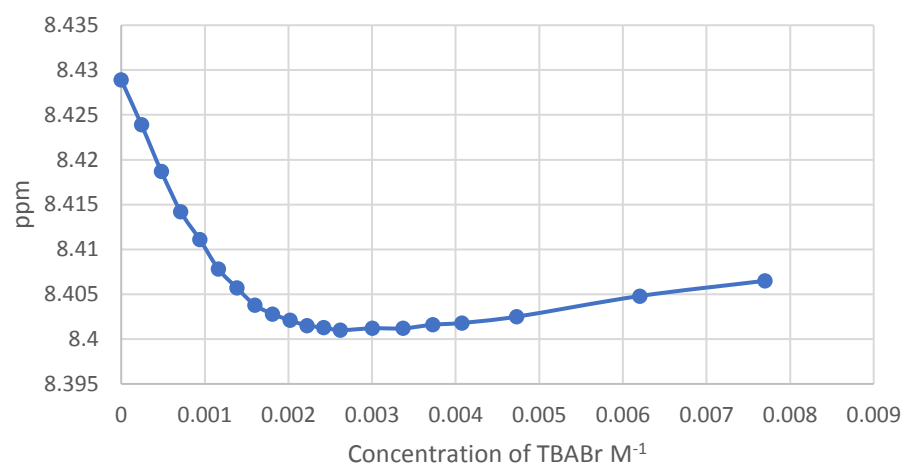
species	S1	D1	S2	D3	D4
H	9.47E+00	9.08E+00	8.45E+00	8.43E+00	8.31E+00
GH	9.40E+00	9.02E+00	8.67E+00	8.39E+00	8.24E+00
G ₂ H	9.46E+00	9.26E+00	8.67E+00	8.43E+00	8.24E+00

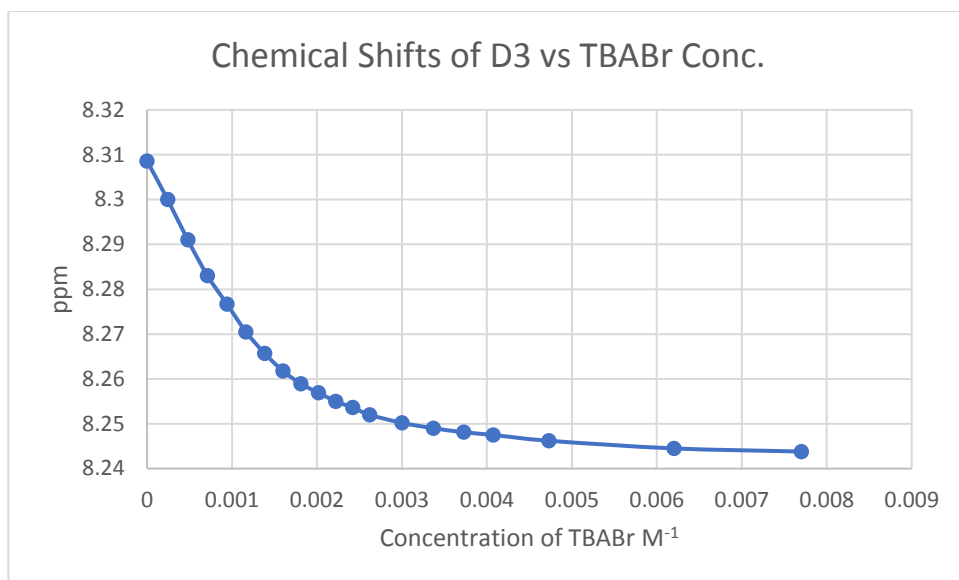


Chemical Shifts of S2 vs TBABr Conc.



Chemical Shifts of D2 vs TBABr Conc.





G1XB and TBA⁺Br⁻ (Experiment 3)

Species	Log beta	G	H	std. dev.
				0.0209
1	3.7667	1	1	
				0.0627
2	5.6408	2	1	

Converged in 1 iterations with sigma = 0.681857

Species concentrations/mol dm⁻³

Point	pH	T(TBABr)	T(G1XB)	F(TBABr)	F(G1XB)	species 1	species 2
1	-	0.00E+00	1.50E-03	6.10E-91	1.50E-03	5.35E-90	2.44E-178
2	-	2.42E-04	1.50E-03	2.82E-05	1.29E-03	2.13E-04	4.50E-07
3	-	4.79E-04	1.50E-03	6.45E-05	1.09E-03	4.11E-04	1.98E-06
4	-	7.12E-04	1.50E-03	1.11E-04	9.07E-04	5.91E-04	4.92E-06
5	-	9.40E-04	1.50E-03	1.72E-04	7.45E-04	7.49E-04	9.64E-06
6	-	1.16E-03	1.50E-03	2.49E-04	6.05E-04	8.82E-04	1.65E-05
7	-	1.38E-03	1.50E-03	3.45E-04	4.90E-04	9.88E-04	2.55E-05
8	-	1.60E-03	1.50E-03	4.58E-04	3.99E-04	1.07E-03	3.66E-05
9	-	1.81E-03	1.50E-03	5.86E-04	3.28E-04	1.13E-03	4.94E-05
10	-	2.02E-03	1.50E-03	7.26E-04	2.75E-04	1.17E-03	6.33E-05
11	-	2.22E-03	1.50E-03	8.74E-04	2.33E-04	1.19E-03	7.80E-05
12	-	2.42E-03	1.50E-03	1.03E-03	2.01E-04	1.21E-03	9.29E-05
13	-	2.62E-03	1.50E-03	1.18E-03	1.76E-04	1.22E-03	1.08E-04
14	-	3.00E-03	1.50E-03	1.50E-03	1.40E-04	1.23E-03	1.38E-04
15	-	3.37E-03	1.50E-03	1.82E-03	1.15E-04	1.22E-03	1.66E-04
16	-	3.73E-03	1.50E-03	2.13E-03	9.74E-05	1.21E-03	1.93E-04
17	-	4.07E-03	1.50E-03	2.44E-03	8.43E-05	1.20E-03	2.19E-04

18	-	4.73E-03	1.50E-03	3.03E-03	6.62E-05	1.17E-03	2.65E-04
19	-	6.20E-03	1.50E-03	4.38E-03	4.30E-05	1.10E-03	3.60E-04
20	-	7.70E-03	1.50E-03	5.78E-03	3.04E-05	1.03E-03	4.45E-04

Measured chemical shifts

Point	pH	S1	D1	S2	D3	D4
1	-	9.47E+00	9.08E+00	8.45E+00	8.43E+00	8.31E+00
2	-	9.46E+00	9.07E+00	8.48E+00	8.43E+00	8.30E+00
3	-	9.45E+00	9.06E+00	8.51E+00	8.42E+00	8.29E+00
4	-	9.45E+00	9.06E+00	8.54E+00	8.42E+00	8.28E+00
5	-	9.44E+00	9.05E+00	8.56E+00	8.41E+00	8.28E+00
6	-	9.43E+00	9.05E+00	8.58E+00	8.41E+00	8.27E+00
7	-	9.43E+00	9.05E+00	8.59E+00	8.41E+00	8.27E+00
8	-	9.43E+00	9.05E+00	8.61E+00	8.40E+00	8.26E+00
9	-	9.42E+00	9.05E+00	8.62E+00	8.40E+00	8.26E+00
10	-	9.42E+00	9.05E+00	8.62E+00	8.40E+00	8.26E+00
11	-	9.42E+00	9.05E+00	8.63E+00	8.40E+00	8.26E+00
12	-	9.42E+00	9.05E+00	8.63E+00	8.40E+00	8.25E+00
13	-	9.42E+00	9.05E+00	8.64E+00	8.40E+00	8.25E+00
14	-	9.42E+00	9.06E+00	8.64E+00	8.40E+00	8.25E+00
15	-	9.42E+00	9.06E+00	8.65E+00	8.40E+00	8.25E+00
16	-	9.42E+00	9.07E+00	8.65E+00	8.40E+00	8.25E+00
17	-	9.42E+00	9.07E+00	8.65E+00	8.40E+00	8.25E+00
18	-	9.42E+00	9.08E+00	8.66E+00	8.40E+00	8.25E+00
19	-	9.42E+00	9.09E+00	8.66E+00	8.40E+00	8.25E+00
20	-	9.42E+00	9.11E+00	8.66E+00	8.41E+00	8.24E+00

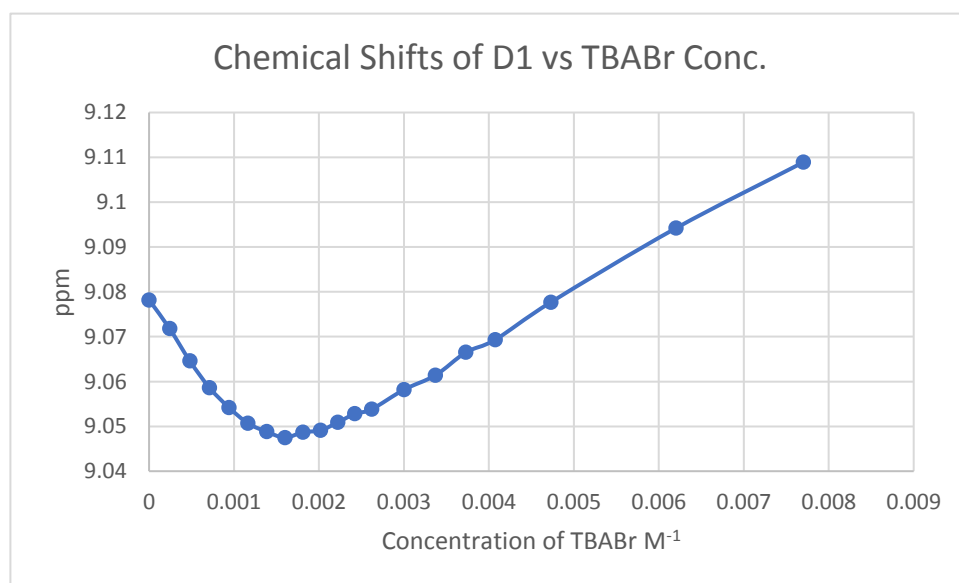
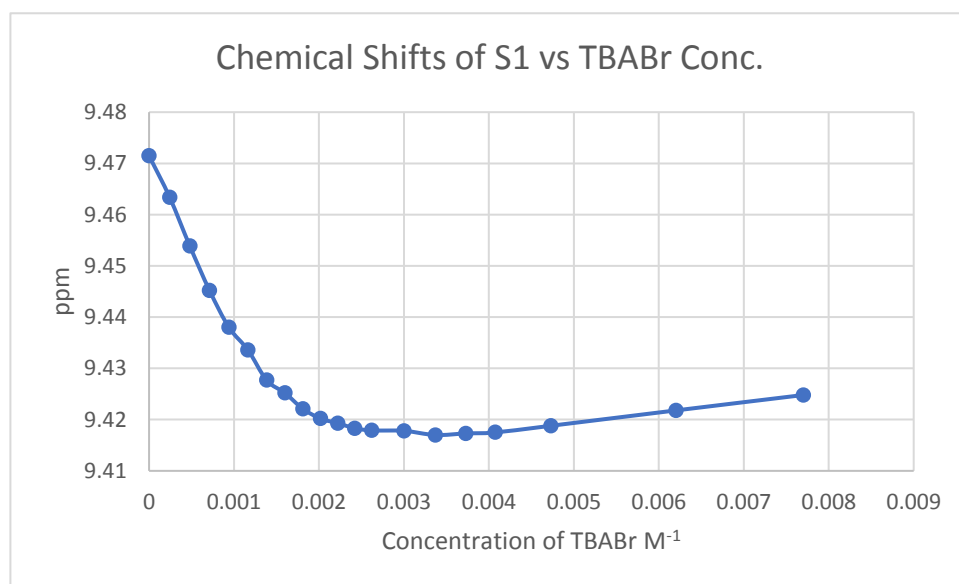
Calculated chemical shifts

Point	pH	S1	D1	S2	D3	D4
1	-	9.47E+00	9.08E+00	8.45E+00	8.43E+00	8.31E+00
2	-	9.46E+00	9.07E+00	8.48E+00	8.42E+00	8.30E+00
3	-	9.45E+00	9.06E+00	8.51E+00	8.42E+00	8.29E+00
4	-	9.45E+00	9.06E+00	8.54E+00	8.42E+00	8.28E+00
5	-	9.44E+00	9.05E+00	8.56E+00	8.41E+00	8.28E+00
6	-	9.43E+00	9.05E+00	8.58E+00	8.41E+00	8.27E+00
7	-	9.43E+00	9.05E+00	8.59E+00	8.41E+00	8.27E+00
8	-	9.42E+00	9.05E+00	8.61E+00	8.40E+00	8.26E+00
9	-	9.42E+00	9.05E+00	8.62E+00	8.40E+00	8.26E+00
10	-	9.42E+00	9.05E+00	8.62E+00	8.40E+00	8.26E+00
11	-	9.42E+00	9.05E+00	8.63E+00	8.40E+00	8.26E+00
12	-	9.42E+00	9.05E+00	8.64E+00	8.40E+00	8.25E+00
13	-	9.42E+00	9.05E+00	8.64E+00	8.40E+00	8.25E+00
14	-	9.42E+00	9.06E+00	8.64E+00	8.40E+00	8.25E+00

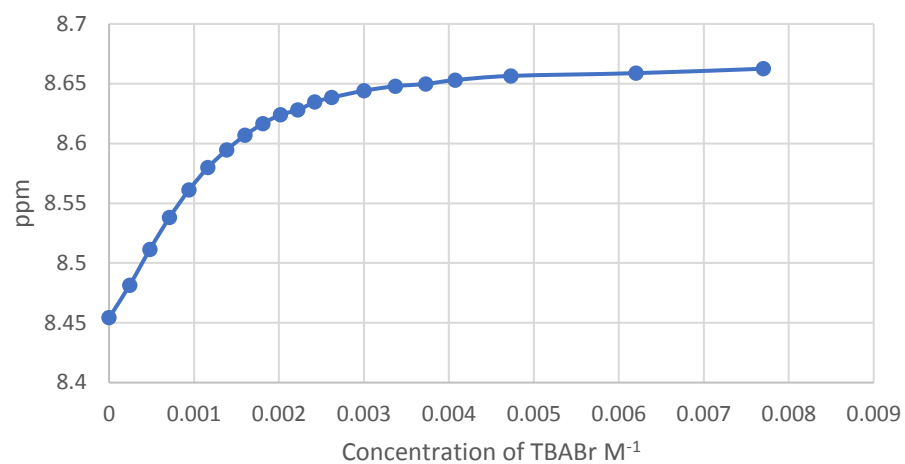
15	-	9.42E+00	9.06E+00	8.65E+00	8.40E+00	8.25E+00
16	-	9.42E+00	9.07E+00	8.65E+00	8.40E+00	8.25E+00
17	-	9.42E+00	9.07E+00	8.65E+00	8.40E+00	8.25E+00
18	-	9.42E+00	9.08E+00	8.66E+00	8.40E+00	8.25E+00
19	-	9.42E+00	9.09E+00	8.66E+00	8.40E+00	8.25E+00
20	-	9.42E+00	9.11E+00	8.66E+00	8.41E+00	8.24E+00

Chemical shifts for each nucleus

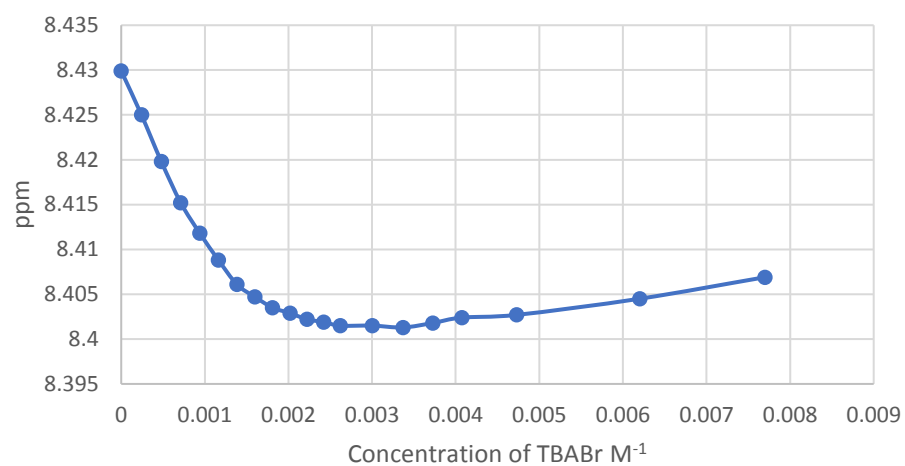
species	S1	D1	S2	D3	D4
H	9.47E+00	9.08E+00	8.45E+00	8.43E+00	8.31E+00
GH	9.41E+00	9.03E+00	8.66E+00	8.39E+00	8.25E+00
G ₂ H	9.46E+00	9.30E+00	8.68E+00	8.43E+00	8.24E+00

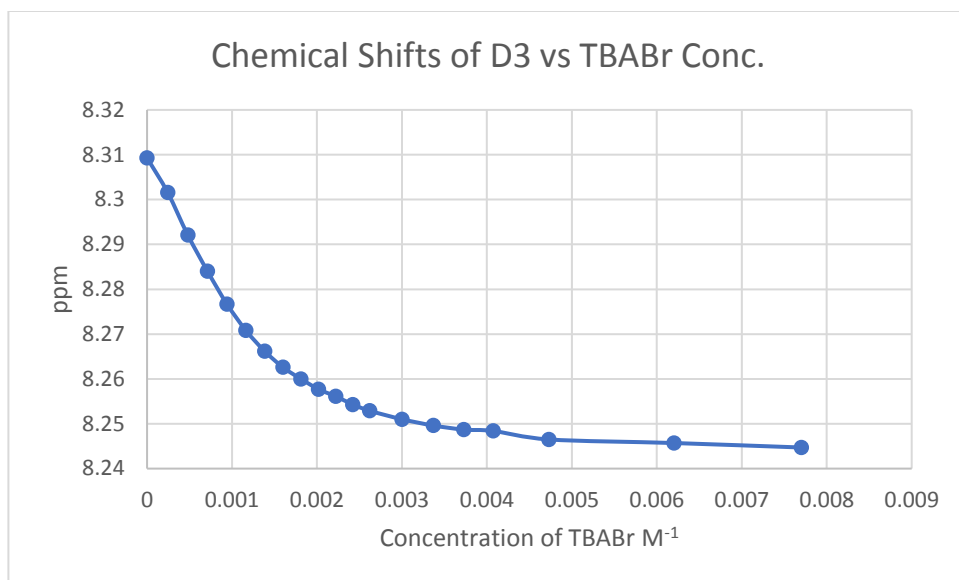


Chemical Shifts of S2 vs TBABr Conc.



Chemical Shifts of D2 vs TBABr Conc.





G1XB and TBA⁺I⁻ (Experiment 1)

Species	Log beta	G	H	std. dev.
				0.0344
1	3.5404	1	1	
2	5.0629	2	1	0.2511

Converged in 1 iterations with sigma = 0.089272

Species concentrations/mol dm⁻³

Point	pH	T(TBAI)	T(G1XB)	F(TBAI)	F(G1XB)	species 1	species 2
1	-	0.00E+00	1.63E-03	8.74E-91	1.63E-03	4.93E-90	1.44E-178
2	-	2.24E-04	1.63E-03	3.73E-05	1.44E-03	1.86E-04	2.32E-07
3	-	4.44E-04	1.63E-03	8.21E-05	1.26E-03	3.60E-04	9.84E-07
4	-	6.60E-04	1.63E-03	1.36E-04	1.10E-03	5.20E-04	2.35E-06
5	-	8.71E-04	1.63E-03	1.99E-04	9.58E-04	6.63E-04	4.40E-06
6	-	1.08E-03	1.63E-03	2.75E-04	8.29E-04	7.90E-04	7.22E-06
7	-	1.28E-03	1.63E-03	3.62E-04	7.16E-04	8.99E-04	1.08E-05
8	-	1.48E-03	1.63E-03	4.61E-04	6.20E-04	9.91E-04	1.52E-05
9	-	1.68E-03	1.63E-03	5.71E-04	5.39E-04	1.07E-03	2.03E-05
10	-	1.87E-03	1.63E-03	6.90E-04	4.71E-04	1.13E-03	2.59E-05
11	-	2.06E-03	1.63E-03	8.17E-04	4.16E-04	1.18E-03	3.21E-05
12	-	2.24E-03	1.63E-03	9.50E-04	3.69E-04	1.22E-03	3.85E-05
13	-	2.43E-03	1.63E-03	1.09E-03	3.31E-04	1.25E-03	4.52E-05
14	-	2.78E-03	1.63E-03	1.37E-03	2.72E-04	1.29E-03	5.90E-05
15	-	3.12E-03	1.63E-03	1.66E-03	2.30E-04	1.32E-03	7.29E-05
16	-	3.78E-03	1.63E-03	2.22E-03	1.75E-04	1.35E-03	1.00E-04
17	-	4.96E-03	1.63E-03	3.30E-03	1.19E-04	1.36E-03	1.49E-04
18	-	6.24E-03	1.63E-03	4.50E-03	8.58E-05	1.34E-03	2.01E-04

19	-	7.35E-03	1.63E-03	5.55E-03	6.83E-05	1.31E-03	2.43E-04
20	-	8.32E-03	1.63E-03	6.47E-03	5.75E-05	1.29E-03	2.78E-04

Measured chemical shifts

Point	pH	S1	D1	S2
1	-	9.47E+00	9.08E+00	8.45E+00
2	-	9.47E+00	9.08E+00	8.47E+00
3	-	9.46E+00	9.07E+00	8.49E+00
4	-	9.45E+00	9.06E+00	8.51E+00
5	-	9.44E+00	9.06E+00	8.53E+00
6	-	9.44E+00	9.05E+00	8.54E+00
7	-	9.43E+00	9.05E+00	8.56E+00
8	-	9.43E+00	9.05E+00	8.57E+00
9	-	9.42E+00	9.05E+00	8.58E+00
10	-	9.42E+00	9.04E+00	8.58E+00
11	-	9.42E+00	9.04E+00	8.59E+00
12	-	9.42E+00	9.04E+00	8.60E+00
13	-	9.41E+00	9.05E+00	8.60E+00
14	-	9.41E+00	9.04E+00	8.61E+00
15	-			
16	-	9.41E+00	9.05E+00	8.62E+00
17	-	9.41E+00	9.05E+00	8.62E+00
18	-	9.41E+00	9.06E+00	8.63E+00
19	-	9.41E+00	9.07E+00	8.63E+00
20	-	9.41E+00	9.07E+00	8.63E+00

Calculated chemical shifts

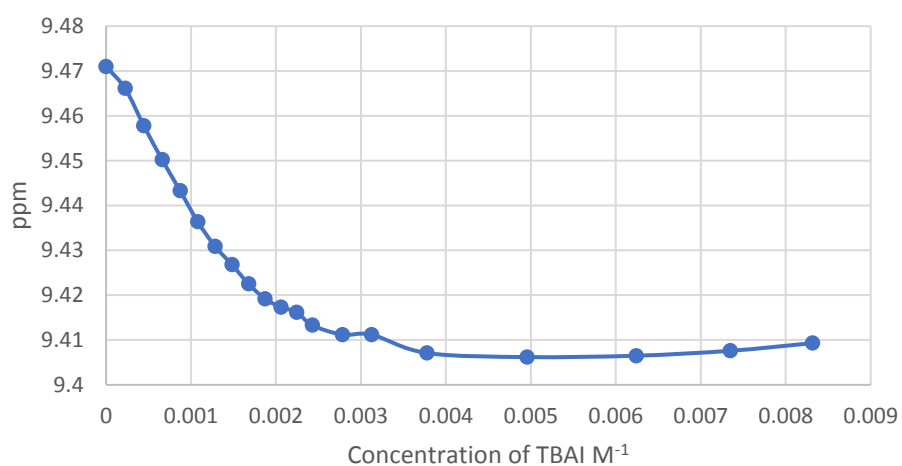
Point	pH	S1	D1	S2
1	-	9.47E+00	9.08E+00	8.45E+00
2	-	9.47E+00	9.07E+00	8.47E+00
3	-	9.46E+00	9.07E+00	8.49E+00
4	-	9.45E+00	9.06E+00	8.51E+00
5	-	9.44E+00	9.06E+00	8.53E+00
6	-	9.44E+00	9.05E+00	8.54E+00
7	-	9.43E+00	9.05E+00	8.56E+00
8	-	9.43E+00	9.05E+00	8.57E+00
9	-	9.42E+00	9.05E+00	8.58E+00
10	-	9.42E+00	9.05E+00	8.58E+00
11	-	9.42E+00	9.04E+00	8.59E+00
12	-	9.42E+00	9.04E+00	8.60E+00
13	-	9.41E+00	9.04E+00	8.60E+00
14	-	9.41E+00	9.04E+00	8.61E+00
15	-			
16	-	9.41E+00	9.05E+00	8.62E+00

17	-	9.41E+00	9.05E+00	8.62E+00
18	-	9.41E+00	9.06E+00	8.63E+00
19	-	9.41E+00	9.07E+00	8.63E+00
20	-	9.41E+00	9.07E+00	8.63E+00

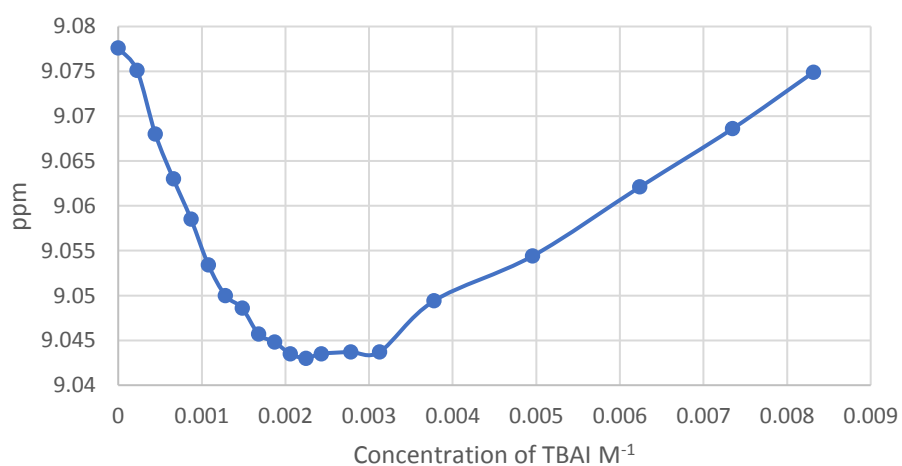
Chemical shifts for each nucleus

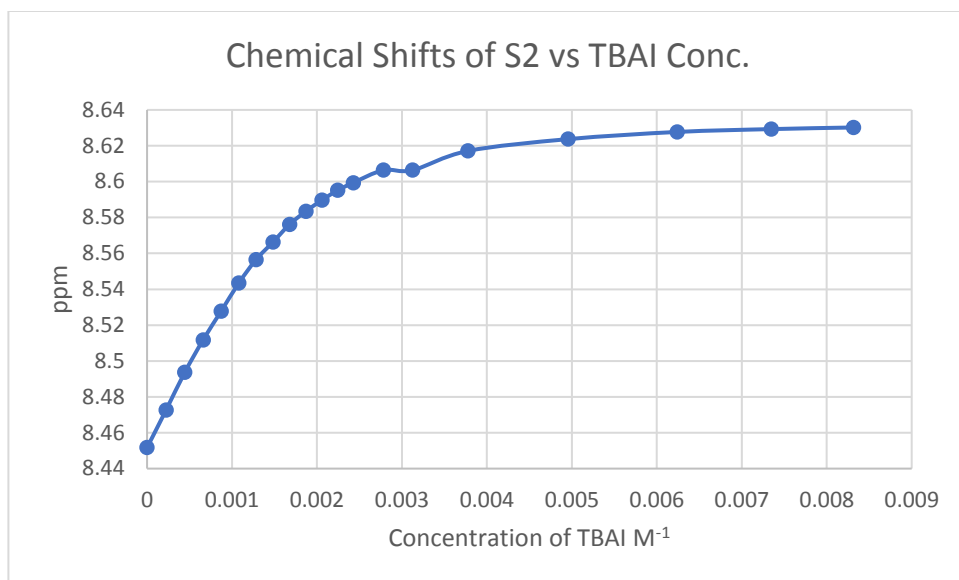
species	S1	D1	S2
H	9.47E+00	9.08E+00	8.45E+00
GH	9.40E+00	9.02E+00	8.64E+00
G ₂ H	9.45E+00	9.31E+00	8.63E+00

Chemical Shifts of S1 vs TBAI Conc.



Chemical Shifts of D1 vs TBAI Conc.





G1XB and TBA⁺I⁻ (Experiment 2)

Species	Log beta	G	H	std. dev.
				0.0313
1	3.7246	1	1	
				0.1533
2	5.4657	2	1	

Converged in 1 iterations with sigma = 0.886927

Species concentrations/mol dm⁻³

Point	pH	T(TBAI)	T(G1XB)	F(TBAI)	F(G1XB)	species 1	species 2
1	-	0.00E+00	1.53E-03	6.54E-91	1.53E-03	5.30E-90	1.91E-178
2	-	2.44E-04	1.53E-03	3.05E-05	1.31E-03	2.12E-04	3.57E-07
3	-	4.83E-04	1.53E-03	6.93E-05	1.12E-03	4.10E-04	1.57E-06
4	-	7.17E-04	1.53E-03	1.19E-04	9.33E-04	5.90E-04	3.87E-06
5	-	9.47E-04	1.53E-03	1.83E-04	7.71E-04	7.49E-04	7.55E-06
6	-	1.17E-03	1.53E-03	2.64E-04	6.32E-04	8.83E-04	1.28E-05
7	-	1.39E-03	1.53E-03	3.62E-04	5.16E-04	9.91E-04	1.98E-05
8	-	1.61E-03	1.53E-03	4.78E-04	4.24E-04	1.08E-03	2.83E-05
9	-	1.82E-03	1.53E-03	6.09E-04	3.52E-04	1.14E-03	3.82E-05
10	-	2.03E-03	1.53E-03	7.52E-04	2.96E-04	1.18E-03	4.90E-05
11	-	2.24E-03	1.53E-03	9.03E-04	2.53E-04	1.21E-03	6.04E-05
12	-	2.44E-03	1.53E-03	1.06E-03	2.20E-04	1.24E-03	7.21E-05
13	-	2.64E-03	1.53E-03	1.22E-03	1.93E-04	1.25E-03	8.40E-05
14	-	3.02E-03	1.53E-03	1.54E-03	1.55E-04	1.27E-03	1.08E-04
15	-	3.39E-03	1.53E-03	1.87E-03	1.28E-04	1.27E-03	1.30E-04
16	-	3.75E-03	1.53E-03	2.18E-03	1.09E-04	1.27E-03	1.52E-04
17	-	4.10E-03	1.53E-03	2.50E-03	9.51E-05	1.26E-03	1.73E-04

18	-	4.76E-03	1.53E-03	3.10E-03	7.54E-05	1.24E-03	2.12E-04
19	-	6.24E-03	1.53E-03	4.48E-03	4.99E-05	1.19E-03	2.92E-04
20	-	7.75E-03	1.53E-03	5.90E-03	3.60E-05	1.13E-03	3.66E-04

Measured chemical shifts

Point	pH	S1	D1	S2
1	-	9.47E+00	9.08E+00	8.45E+00
2	-	9.46E+00	9.07E+00	8.48E+00
3	-	9.45E+00	9.06E+00	8.50E+00
4	-	9.44E+00	9.06E+00	8.53E+00
5	-	9.43E+00	9.05E+00	8.55E+00
6	-	9.43E+00	9.05E+00	8.56E+00
7	-	9.42E+00	9.04E+00	8.57E+00
8	-	9.42E+00	9.04E+00	8.58E+00
9	-	9.41E+00	9.04E+00	8.59E+00
10	-	9.41E+00	9.04E+00	8.60E+00
11	-	9.41E+00	9.04E+00	8.60E+00
12	-	9.41E+00	9.04E+00	8.61E+00
13	-	9.41E+00	9.04E+00	8.61E+00
14	-	9.40E+00	9.04E+00	8.62E+00
15	-	9.40E+00	9.05E+00	8.62E+00
16	-	9.40E+00	9.05E+00	8.62E+00
17	-	9.40E+00	9.05E+00	8.62E+00
18	-	9.40E+00	9.06E+00	8.63E+00
19	-	9.40E+00	9.07E+00	8.63E+00
20	-	9.41E+00	9.08E+00	8.63E+00

Calculated chemical shifts

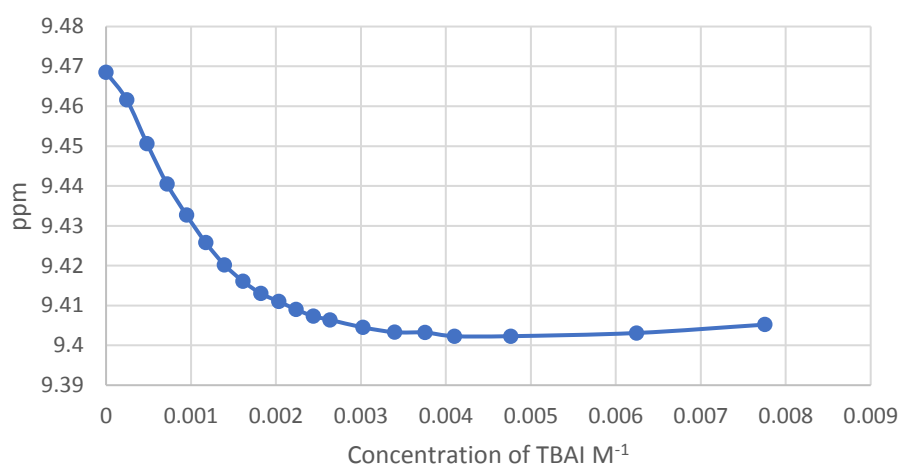
Point	pH	S1	D1	S2
1	-	9.47E+00	9.08E+00	8.45E+00
2	-	9.46E+00	9.07E+00	8.48E+00
3	-	9.45E+00	9.06E+00	8.50E+00
4	-	9.44E+00	9.06E+00	8.52E+00
5	-	9.43E+00	9.05E+00	8.54E+00
6	-	9.43E+00	9.05E+00	8.56E+00
7	-	9.42E+00	9.04E+00	8.57E+00
8	-	9.42E+00	9.04E+00	8.58E+00
9	-	9.41E+00	9.04E+00	8.59E+00
10	-	9.41E+00	9.04E+00	8.60E+00
11	-	9.41E+00	9.04E+00	8.60E+00
12	-	9.41E+00	9.04E+00	8.61E+00
13	-	9.41E+00	9.04E+00	8.61E+00
14	-	9.40E+00	9.04E+00	8.62E+00
15	-	9.40E+00	9.05E+00	8.62E+00

16	-	9.40E+00	9.05E+00	8.62E+00
17	-	9.40E+00	9.05E+00	8.62E+00
18	-	9.40E+00	9.06E+00	8.63E+00
19	-	9.40E+00	9.07E+00	8.63E+00
20	-	9.40E+00	9.08E+00	8.63E+00

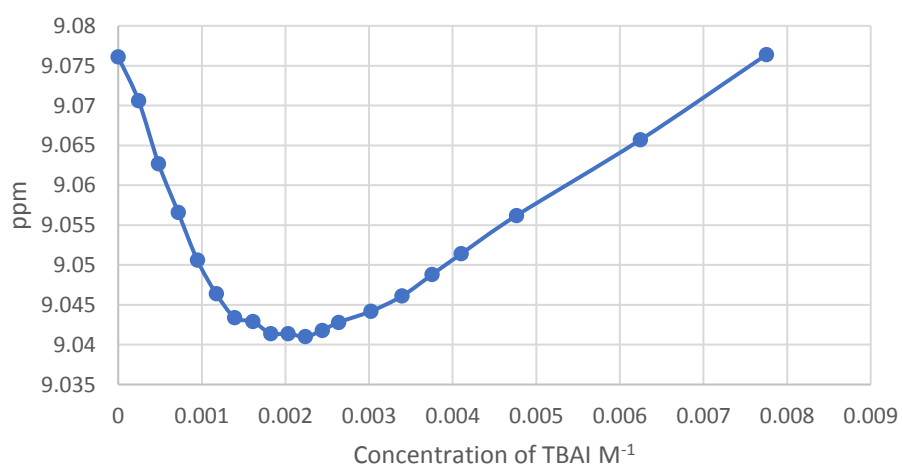
Chemical shifts for each nucleus

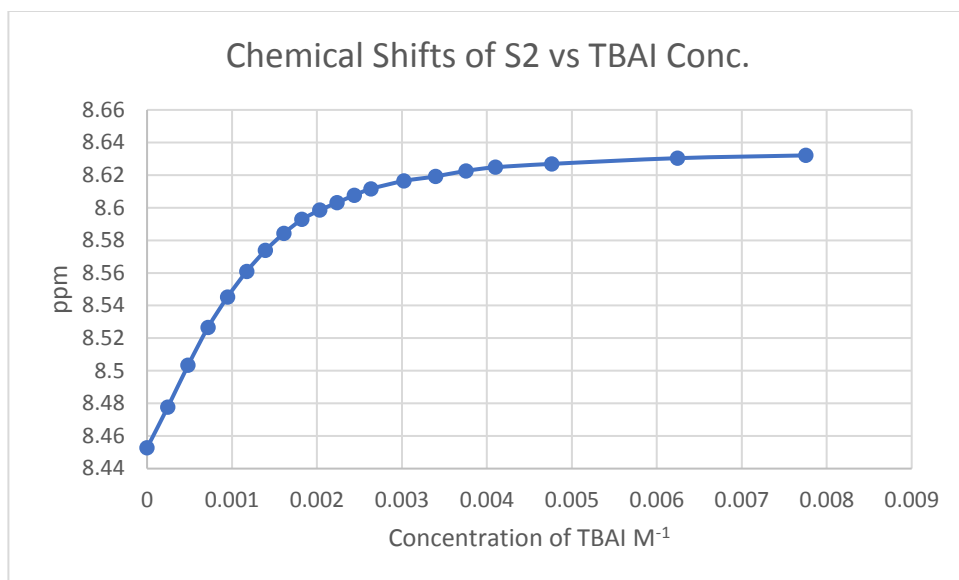
species	S1	D1	S2
H	9.47E+00	9.08E+00	8.45E+00
GH	9.39E+00	9.02E+00	8.63E+00
G ₂ H	9.43E+00	9.24E+00	8.64E+00

Chemical Shifts of S1 vs TBAI Conc.



Chemical Shifts of D1 vs TBAI Conc.





G1XB and TBAI⁺I⁻ (Experiment 3)

Species	Log beta	G	H	std. dev.
				0.027
1	3.6605	1	1	
2	5.2304	2	1	0.1838

Converged in 1 iterations with sigma = 0.793999

Species concentrations/mol dm⁻³

Point	pH	T(TBAI)	T(G1XB)	F(TBAI)	F(G1XB)	species 1	species 2
1	-	0.00E+00	1.53E-03	7.17E-91	1.53E-03	5.01E-90	1.34E-178
2	-	2.44E-04	1.53E-03	3.46E-05	1.32E-03	2.09E-04	2.68E-07
3	-	4.83E-04	1.53E-03	7.82E-05	1.12E-03	4.02E-04	1.17E-06
4	-	7.17E-04	1.53E-03	1.33E-04	9.47E-04	5.78E-04	2.86E-06
5	-	9.47E-04	1.53E-03	2.03E-04	7.89E-04	7.33E-04	5.52E-06
6	-	1.17E-03	1.53E-03	2.89E-04	6.54E-04	8.64E-04	9.28E-06
7	-	1.39E-03	1.53E-03	3.93E-04	5.41E-04	9.72E-04	1.42E-05
8	-	1.61E-03	1.53E-03	5.13E-04	4.50E-04	1.06E-03	2.01E-05
9	-	1.82E-03	1.53E-03	6.47E-04	3.79E-04	1.12E-03	2.70E-05
10	-	2.03E-03	1.53E-03	7.93E-04	3.23E-04	1.17E-03	3.45E-05
11	-	2.24E-03	1.53E-03	9.46E-04	2.79E-04	1.21E-03	4.24E-05
12	-	2.44E-03	1.53E-03	1.11E-03	2.44E-04	1.23E-03	5.06E-05
13	-	2.64E-03	1.53E-03	1.27E-03	2.16E-04	1.25E-03	5.89E-05
14	-	3.02E-03	1.53E-03	1.59E-03	1.75E-04	1.28E-03	7.56E-05
15	-	3.39E-03	1.53E-03	1.92E-03	1.47E-04	1.29E-03	9.20E-05
16	-	3.75E-03	1.53E-03	2.25E-03	1.26E-04	1.29E-03	1.08E-04
17	-	4.10E-03	1.53E-03	2.56E-03	1.10E-04	1.29E-03	1.23E-04
18	-	4.76E-03	1.53E-03	3.17E-03	8.86E-05	1.29E-03	1.52E-04

19	-	6.24E-03	1.53E-03	4.56E-03	6.01E-05	1.25E-03	2.13E-04
20	-	7.75E-03	1.53E-03	6.00E-03	4.42E-05	1.21E-03	2.70E-04

Measured chemical shifts

Point	pH	S1	D1	S2
1	-	9.47E+00	9.08E+00	8.45E+00
2	-	9.46E+00	9.07E+00	8.48E+00
3	-	9.45E+00	9.07E+00	8.50E+00
4	-	9.44E+00	9.06E+00	8.52E+00
5	-	9.44E+00	9.05E+00	8.54E+00
6	-	9.43E+00	9.05E+00	8.56E+00
7	-	9.42E+00	9.05E+00	8.57E+00
8	-	9.42E+00	9.04E+00	8.58E+00
9	-	9.42E+00	9.04E+00	8.59E+00
10	-	9.41E+00	9.04E+00	8.60E+00
11	-	9.41E+00	9.04E+00	8.60E+00
12	-	9.41E+00	9.04E+00	8.61E+00
13	-	9.41E+00	9.04E+00	8.61E+00
14	-	9.41E+00	9.04E+00	8.61E+00
15	-	9.41E+00	9.05E+00	8.62E+00
16	-	9.40E+00	9.05E+00	8.62E+00
17	-	9.40E+00	9.05E+00	8.62E+00
18	-	9.40E+00	9.06E+00	8.63E+00
19	-	9.40E+00	9.07E+00	8.63E+00
20	-	9.41E+00	9.08E+00	8.63E+00

Calculated chemical shifts

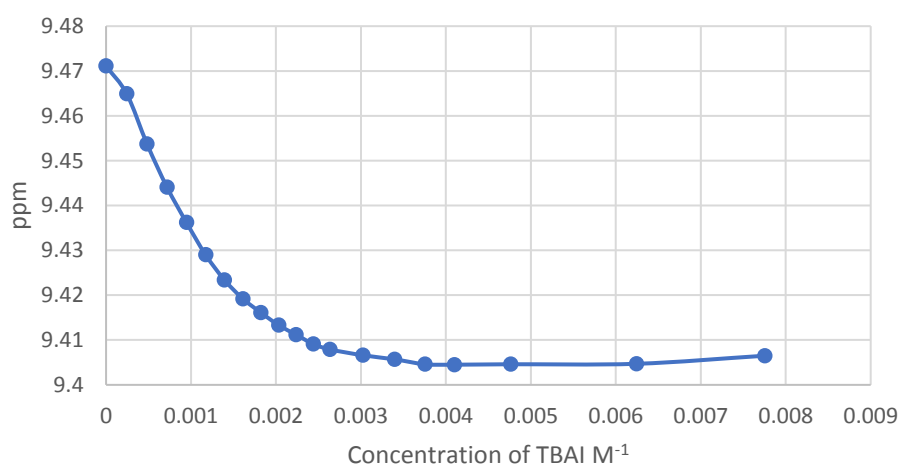
Point	pH	S1	D1	S2
1	-	9.47E+00	9.08E+00	8.45E+00
2	-	9.46E+00	9.07E+00	8.48E+00
3	-	9.45E+00	9.06E+00	8.50E+00
4	-	9.44E+00	9.06E+00	8.52E+00
5	-	9.44E+00	9.05E+00	8.54E+00
6	-	9.43E+00	9.05E+00	8.56E+00
7	-	9.42E+00	9.05E+00	8.57E+00
8	-	9.42E+00	9.04E+00	8.58E+00
9	-	9.42E+00	9.04E+00	8.59E+00
10	-	9.41E+00	9.04E+00	8.60E+00
11	-	9.41E+00	9.04E+00	8.60E+00
12	-	9.41E+00	9.04E+00	8.61E+00
13	-	9.41E+00	9.04E+00	8.61E+00
14	-	9.41E+00	9.04E+00	8.61E+00
15	-	9.41E+00	9.05E+00	8.62E+00
16	-	9.41E+00	9.05E+00	8.62E+00

17	-	9.40E+00	9.05E+00	8.62E+00
18	-	9.40E+00	9.06E+00	8.63E+00
19	-	9.40E+00	9.07E+00	8.63E+00
20	-	9.41E+00	9.08E+00	8.63E+00

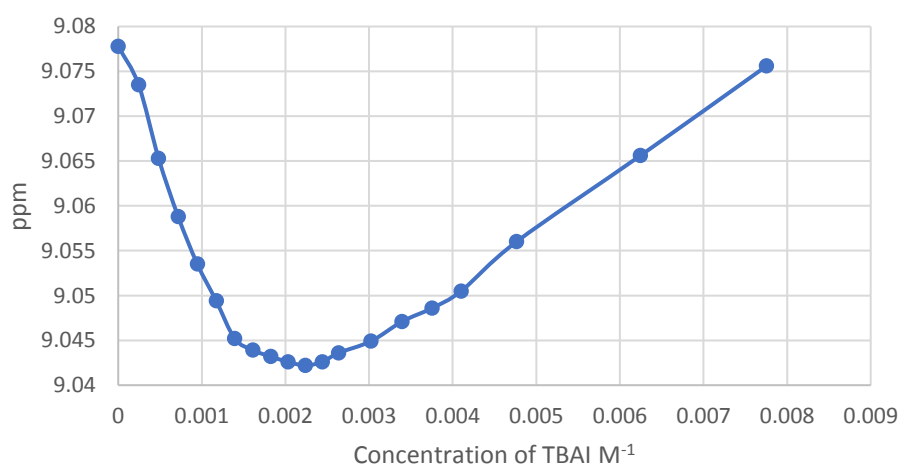
Chemical shifts for each nucleus

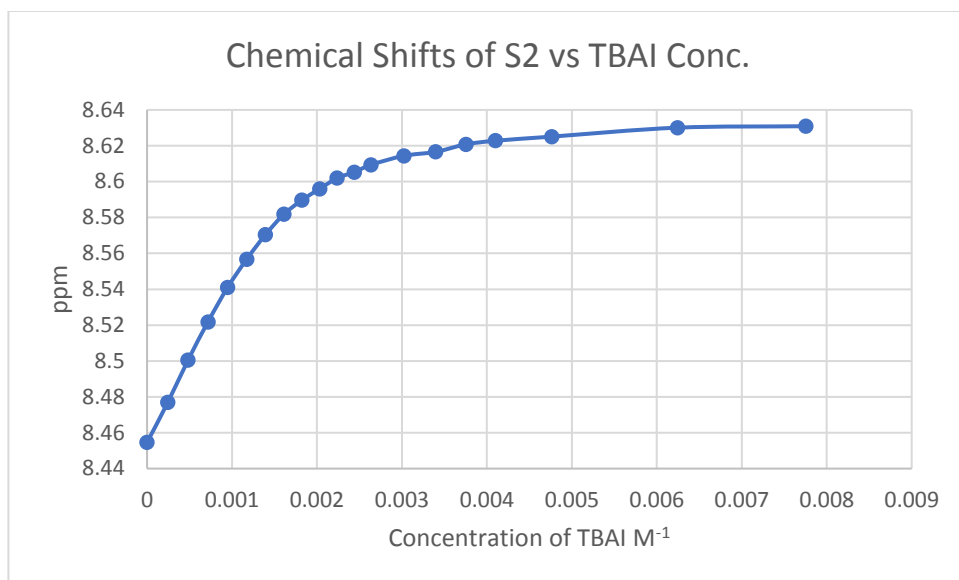
species	S1	D1	S2
H	9.47E+00	9.08E+00	8.45E+00
GH	9.40E+00	9.02E+00	8.63E+00
G ₂ H	9.44E+00	9.30E+00	8.65E+00

Chemical Shifts of S1 vs TBAI Conc.



Chemical Shifts of D1 vs TBAI Conc.





G2HB and TBA⁺Cl⁻ (Experiment 1)

Species	Log beta	G	H	std. dev.
1	3.4477	1	1	0.1037
2	5.7534	2	1	0.1844

Converged in 9 iterations with sigma = 0.137009

Species concentrations/mol dm⁻³

Point	pH	T(TBACl)	T(G2HB)	F(TBACl)	F(G2HB)	species 1	species 2
1	-	0.00E+00	1.46E-03	9.33E-91	1.46E-03	3.81E-90	7.19E-178
2	-	1.67E-04	1.46E-03	3.49E-05	1.33E-03	1.30E-04	9.17E-07
3	-	3.30E-04	1.46E-03	7.37E-05	1.21E-03	2.49E-04	3.71E-06
4	-	4.90E-04	1.46E-03	1.17E-04	1.09E-03	3.57E-04	8.41E-06
5	-	6.47E-04	1.46E-03	1.64E-04	9.89E-04	4.54E-04	1.50E-05
6	-	8.01E-04	1.46E-03	2.15E-04	8.95E-04	5.39E-04	2.35E-05
7	-	9.53E-04	1.46E-03	2.71E-04	8.10E-04	6.15E-04	3.36E-05
8	-	1.10E-03	1.46E-03	3.31E-04	7.33E-04	6.79E-04	4.54E-05
9	-	1.25E-03	1.46E-03	3.95E-04	6.64E-04	7.35E-04	5.86E-05
10	-	1.39E-03	1.46E-03	4.62E-04	6.03E-04	7.81E-04	7.30E-05
11	-	1.53E-03	1.46E-03	5.33E-04	5.49E-04	8.20E-04	8.84E-05
12	-	1.67E-03	1.46E-03	6.07E-04	5.01E-04	8.52E-04	1.05E-04
13	-	1.80E-03	1.46E-03	6.83E-04	4.59E-04	8.78E-04	1.21E-04
14	-	2.07E-03	1.46E-03	8.41E-04	3.88E-04	9.14E-04	1.56E-04
15	-	2.32E-03	1.46E-03	1.01E-03	3.32E-04	9.36E-04	1.90E-04

16	-	2.81E-03	1.46E-03	1.34E-03	2.52E-04	9.48E-04	2.57E-04
17	-	3.26E-03	1.46E-03	1.68E-03	1.99E-04	9.39E-04	3.19E-04
18	-	5.14E-03	1.46E-03	3.24E-03	9.11E-05	8.26E-04	5.40E-04
19	-	6.57E-03	1.46E-03	4.50E-03	5.81E-05	7.33E-04	6.67E-04
20	-	7.68E-03	1.46E-03	5.52E-03	4.32E-05	6.68E-04	7.46E-04

Measured chemical shifts

Point	pH	D1	D2
1	-	9.05E+00	8.47E+00
2	-	9.05E+00	8.48E+00
3	-	9.06E+00	8.50E+00
4	-	9.06E+00	8.51E+00
5	-	9.07E+00	8.53E+00
6	-	9.07E+00	8.55E+00
7	-	9.07E+00	8.56E+00
8	-	9.08E+00	8.57E+00
9	-	9.08E+00	8.58E+00
10	-	9.08E+00	8.59E+00
11	-	9.08E+00	8.60E+00
12	-	9.09E+00	8.61E+00
13	-	9.09E+00	8.62E+00
14	-	9.10E+00	8.63E+00
15	-	9.10E+00	8.64E+00
16	-	9.11E+00	8.65E+00
17	-	9.11E+00	8.66E+00
18	-	9.14E+00	8.69E+00
19	-	9.15E+00	8.70E+00
20	-	9.16E+00	8.70E+00

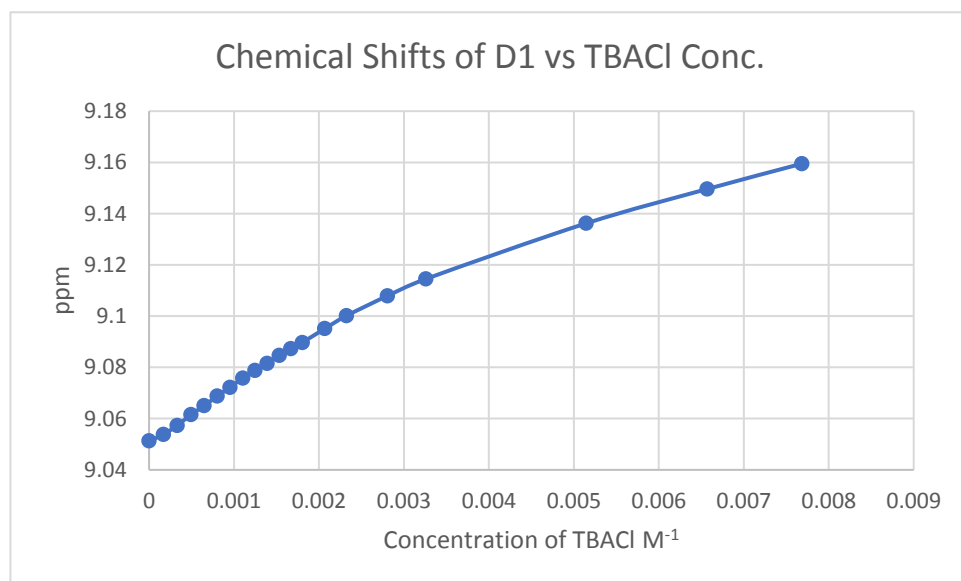
Calculated chemical shifts

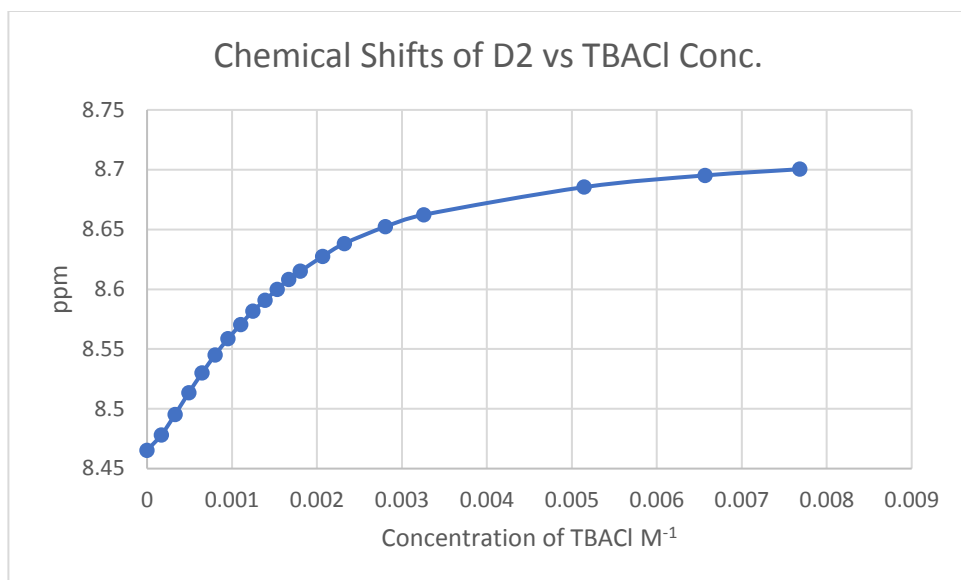
Point	pH	D1	D2
1	-	9.05E+00	8.46E+00
2	-	9.05E+00	8.48E+00
3	-	9.06E+00	8.50E+00
4	-	9.06E+00	8.52E+00
5	-	9.07E+00	8.53E+00
6	-	9.07E+00	8.55E+00
7	-	9.07E+00	8.56E+00
8	-	9.08E+00	8.57E+00
9	-	9.08E+00	8.58E+00
10	-	9.08E+00	8.59E+00
11	-	9.08E+00	8.60E+00
12	-	9.09E+00	8.61E+00
13	-	9.09E+00	8.62E+00

14	-	9.10E+00	8.63E+00
15	-	9.10E+00	8.64E+00
16	-	9.11E+00	8.65E+00
17	-	9.12E+00	8.66E+00
18	-	9.14E+00	8.69E+00
19	-	9.15E+00	8.70E+00
20	-	9.16E+00	8.70E+00

Chemical shifts for each nucleus

species	D1	D2
H	9.05E+00	8.46E+00
GH	9.09E+00	8.68E+00
G ₂ H	9.22E+00	8.73E+00





G2HB and TBA⁺Cl⁻ (Experiment 2)

Species	Log beta	G	H	std. dev.
				0.1057
1	3.3394	1	1	
				0.2195
2	5.5367	2	1	

Converged in 1 iterations with sigma = 1.581616

Species concentrations/mol dm⁻³

Point	pH	T(TBACl)	T(G2HB)	F(TBACl)	F(G2HB)	species 1	species 2
1	-	0.00E+00	1.46E-03	1.07E-90	1.46E-03	3.40E-90	5.71E-178
2	-	2.32E-04	1.46E-03	5.99E-05	1.29E-03	1.69E-04	1.59E-06
3	-	4.60E-04	1.46E-03	1.28E-04	1.14E-03	3.19E-04	6.43E-06
4	-	6.83E-04	1.46E-03	2.05E-04	9.99E-04	4.48E-04	1.45E-05
5	-	9.02E-04	1.46E-03	2.91E-04	8.78E-04	5.59E-04	2.57E-05
6	-	1.12E-03	1.46E-03	3.86E-04	7.72E-04	6.51E-04	3.96E-05
7	-	1.33E-03	1.46E-03	4.89E-04	6.80E-04	7.26E-04	5.59E-05
8	-	1.53E-03	1.46E-03	5.99E-04	6.01E-04	7.87E-04	7.42E-05
9	-	1.74E-03	1.46E-03	7.15E-04	5.34E-04	8.34E-04	9.39E-05
10	-	1.94E-03	1.46E-03	8.36E-04	4.77E-04	8.71E-04	1.15E-04
11	-	2.13E-03	1.46E-03	9.61E-04	4.28E-04	8.98E-04	1.36E-04
12	-	2.32E-03	1.46E-03	1.09E-03	3.86E-04	9.19E-04	1.58E-04
13	-	2.51E-03	1.46E-03	1.22E-03	3.50E-04	9.33E-04	1.79E-04
14	-	2.88E-03	1.46E-03	1.49E-03	2.92E-04	9.48E-04	2.22E-04

15	-	3.23E-03	1.46E-03	1.76E-03	2.48E-04	9.51E-04	2.63E-04
16	-	3.58E-03	1.46E-03	2.03E-03	2.14E-04	9.46E-04	3.02E-04
17	-	3.91E-03	1.46E-03	2.29E-03	1.87E-04	9.37E-04	3.38E-04
18	-	4.54E-03	1.46E-03	2.82E-03	1.48E-04	9.10E-04	4.04E-04
19	-	5.95E-03	1.46E-03	4.05E-03	9.44E-05	8.35E-04	5.33E-04
20	-	7.39E-03	1.46E-03	5.35E-03	6.49E-05	7.58E-04	6.39E-04

Measured chemical shifts

Point	pH	D1	D2
1	-	9.05E+00	8.46E+00
2	-	9.05E+00	8.48E+00
3	-	9.06E+00	8.51E+00
4	-	9.06E+00	8.53E+00
5	-	9.07E+00	8.55E+00
6	-	9.07E+00	8.57E+00
7	-	9.08E+00	8.58E+00
8	-	9.08E+00	8.60E+00
9	-	9.09E+00	8.61E+00
10	-	9.09E+00	8.62E+00
11	-	9.09E+00	8.63E+00
12	-	9.10E+00	8.63E+00
13	-	9.10E+00	8.64E+00
14	-	9.11E+00	8.65E+00
15	-	9.11E+00	8.66E+00
16	-	9.11E+00	8.66E+00
17	-	9.12E+00	8.67E+00
18	-	9.13E+00	8.68E+00
19	-	9.14E+00	8.69E+00
20	-	9.15E+00	8.70E+00

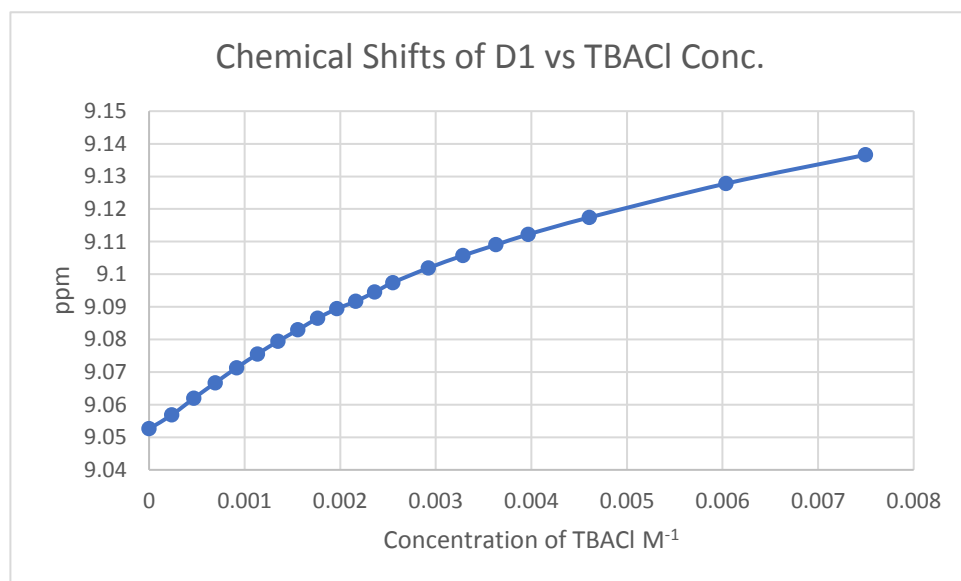
Calculated chemical shifts

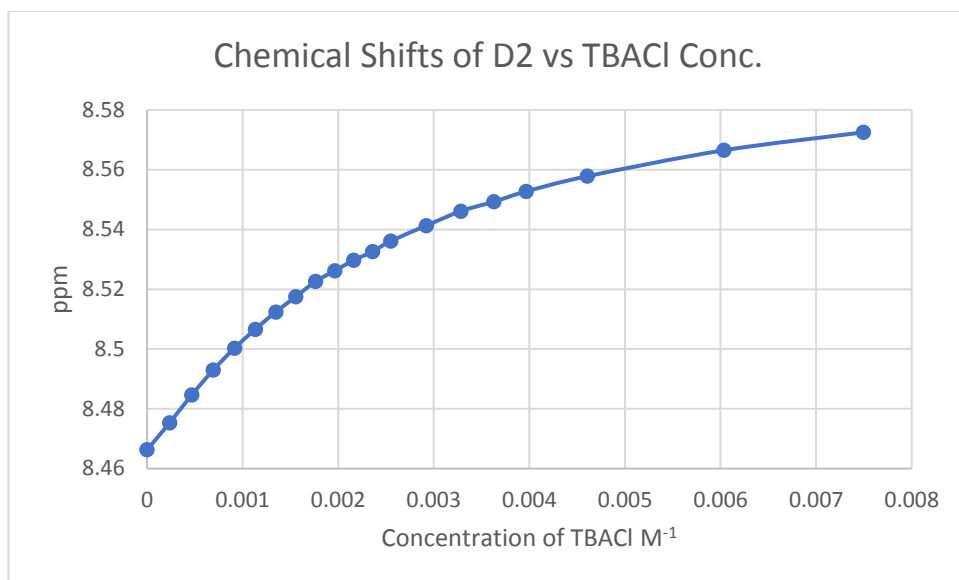
Point	pH	D1	D2
1	-	9.05E+00	8.46E+00
2	-	9.06E+00	8.49E+00
3	-	9.06E+00	8.51E+00
4	-	9.06E+00	8.53E+00
5	-	9.07E+00	8.55E+00
6	-	9.07E+00	8.57E+00
7	-	9.08E+00	8.58E+00
8	-	9.08E+00	8.60E+00
9	-	9.09E+00	8.61E+00
10	-	9.09E+00	8.62E+00
11	-	9.09E+00	8.62E+00

12	-	9.10E+00	8.63E+00
13	-	9.10E+00	8.64E+00
14	-	9.11E+00	8.65E+00
15	-	9.11E+00	8.66E+00
16	-	9.11E+00	8.66E+00
17	-	9.12E+00	8.67E+00
18	-	9.13E+00	8.68E+00
19	-	9.14E+00	8.69E+00
20	-	9.15E+00	8.70E+00

Chemical shifts for each nucleus

species	D1	D2
H	9.05E+00	8.46E+00
GH	9.09E+00	8.69E+00
G ₂ H	9.23E+00	8.73E+00





G2HB and TBA⁺Cl⁻ (Experiment 3)

Species	Log beta	G	H	std. dev.
1	3.4081	1	1	0.1526
2	5.775	2	1	0.2441

Converged in 1 iterations with sigma = 0.183316

Species concentrations/mol dm⁻³

Point	pH	T(TBACl)	T(G2HB)	F(TBACl)	F(G2HB)	species 1	species 2
1	-	0.00E+00	1.46E-03	9.81E-91	1.46E-03	3.67E-90	8.38E-178
2	-	2.32E-04	1.46E-03	5.31E-05	1.29E-03	1.75E-04	2.16E-06
3	-	4.60E-04	1.46E-03	1.14E-04	1.13E-03	3.28E-04	8.71E-06
4	-	6.83E-04	1.46E-03	1.83E-04	9.82E-04	4.60E-04	1.96E-05
5	-	9.02E-04	1.46E-03	2.61E-04	8.56E-04	5.71E-04	3.47E-05
6	-	1.12E-03	1.46E-03	3.47E-04	7.46E-04	6.62E-04	5.35E-05
7	-	1.33E-03	1.46E-03	4.41E-04	6.51E-04	7.35E-04	7.54E-05
8	-	1.53E-03	1.46E-03	5.42E-04	5.71E-04	7.92E-04	9.99E-05
9	-	1.74E-03	1.46E-03	6.50E-04	5.02E-04	8.34E-04	1.26E-04
10	-	1.94E-03	1.46E-03	7.63E-04	4.43E-04	8.65E-04	1.54E-04
11	-	2.13E-03	1.46E-03	8.81E-04	3.93E-04	8.87E-04	1.82E-04
12	-	2.32E-03	1.46E-03	1.00E-03	3.51E-04	9.01E-04	2.10E-04
13	-	2.51E-03	1.46E-03	1.13E-03	3.15E-04	9.09E-04	2.38E-04
14	-	2.88E-03	1.46E-03	1.38E-03	2.58E-04	9.11E-04	2.93E-04
15	-	3.23E-03	1.46E-03	1.64E-03	2.15E-04	9.02E-04	3.45E-04
16	-	3.58E-03	1.46E-03	1.90E-03	1.82E-04	8.87E-04	3.93E-04

17	-	3.91E-03	1.46E-03	2.16E-03	1.57E-04	8.68E-04	4.37E-04
18	-	4.54E-03	1.46E-03	2.68E-03	1.20E-04	8.26E-04	5.15E-04
19	-	5.95E-03	1.46E-03	3.90E-03	7.30E-05	7.28E-04	6.61E-04
20	-	7.39E-03	1.46E-03	5.20E-03	4.81E-05	6.40E-04	7.74E-04

Measured chemical shifts

Point	pH	D1	D2
1	-	9.05E+00	8.47E+00
2	-	9.06E+00	8.48E+00
3	-	9.06E+00	8.50E+00
4	-	9.06E+00	8.52E+00
5	-	9.07E+00	8.54E+00
6	-	9.07E+00	8.56E+00
7	-	9.08E+00	8.58E+00
8	-	9.08E+00	8.59E+00
9	-	9.09E+00	8.60E+00
10	-	9.09E+00	8.61E+00
11	-	9.09E+00	8.62E+00
12	-	9.10E+00	8.63E+00
13	-	9.10E+00	8.63E+00
14	-	9.10E+00	8.64E+00
15	-	9.11E+00	8.65E+00
16	-	9.11E+00	8.66E+00
17	-	9.12E+00	8.67E+00
18	-	9.12E+00	8.67E+00
19	-	9.14E+00	8.69E+00
20	-	9.15E+00	8.70E+00

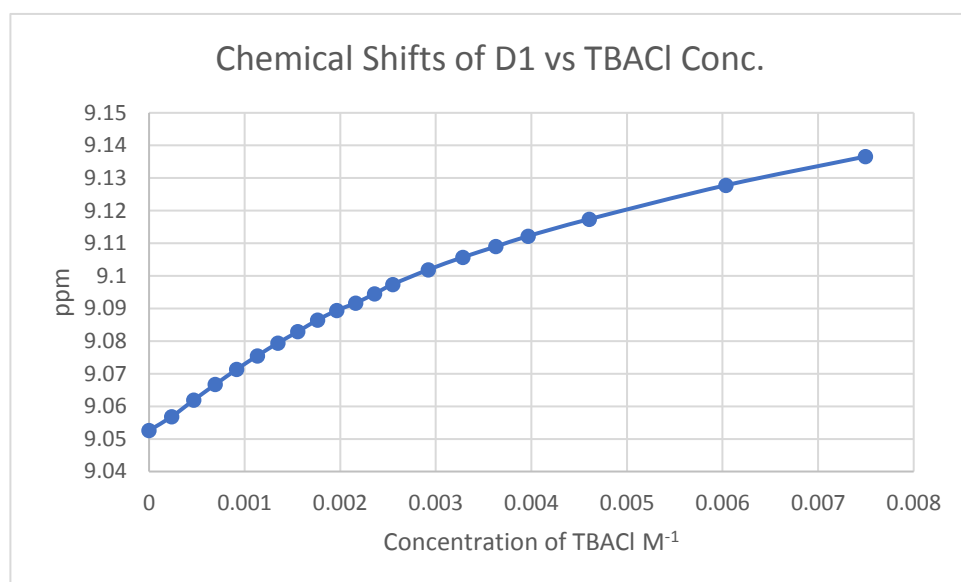
Calculated chemical shifts

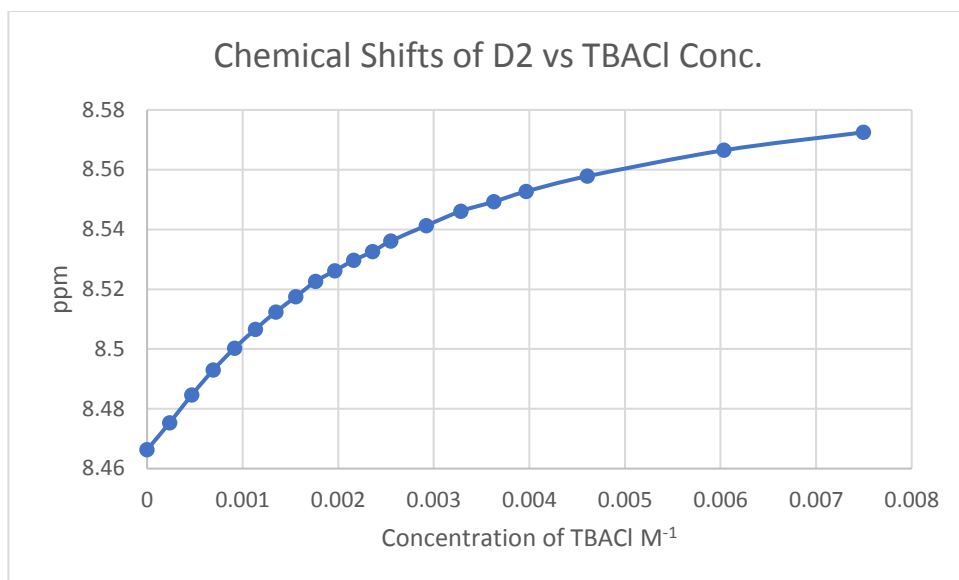
Point	pH	D1	D2
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2	-	9.06E+00	8.48E+00
3	-	9.06E+00	8.51E+00
4	-	9.06E+00	8.53E+00
5	-	9.07E+00	8.55E+00
6	-	9.07E+00	8.56E+00
7	-	9.08E+00	8.58E+00
8	-	9.08E+00	8.59E+00
9	-	9.09E+00	8.60E+00
10	-	9.09E+00	8.61E+00

11	-	9.09E+00	8.62E+00
12	-	9.10E+00	8.63E+00
13	-	9.10E+00	8.63E+00
14	-	9.10E+00	8.64E+00
15	-	9.11E+00	8.65E+00
16	-	9.11E+00	8.66E+00
17	-	9.12E+00	8.67E+00
18	-	9.13E+00	8.67E+00
19	-	9.14E+00	8.69E+00
20	-	9.15E+00	8.70E+00

Chemical shifts for each nucleus

species	D1	D2
H	9.05E+00	8.46E+00
GH	9.09E+00	8.67E+00
G ₂ H	9.21E+00	8.74E+00





G2HB and TBA⁺Br⁻ (Experiment 1)

Species	Log beta	G	H	std. dev.
				0.0651
1	3.3158	1	1	
				0.1388
2	5.3242	2	1	

Converged in 1 iterations with sigma = 0.064735

Species concentrations/mol dm⁻³

Point	pH	T(TBABr)	T(G2HB)	F(TBABr)	F(G2HB)	species 1	species 2
1	-	0.00E+00	1.50E-03	1.11E-90	1.50E-03	3.44E-90	3.89E-178
2	-	1.78E-04	1.50E-03	4.63E-05	1.37E-03	1.31E-04	6.17E-07
3	-	3.53E-04	1.50E-03	9.74E-05	1.24E-03	2.51E-04	2.49E-06
4	-	5.25E-04	1.50E-03	1.54E-04	1.13E-03	3.60E-04	5.63E-06
5	-	6.93E-04	1.50E-03	2.15E-04	1.03E-03	4.58E-04	1.00E-05
6	-	8.58E-04	1.50E-03	2.81E-04	9.36E-04	5.45E-04	1.56E-05
7	-	1.02E-03	1.50E-03	3.53E-04	8.53E-04	6.22E-04	2.24E-05
8	-	1.18E-03	1.50E-03	4.29E-04	7.78E-04	6.90E-04	3.01E-05
9	-	1.33E-03	1.50E-03	5.09E-04	7.10E-04	7.48E-04	3.88E-05
10	-	1.49E-03	1.50E-03	5.93E-04	6.51E-04	7.98E-04	4.82E-05
11	-	1.64E-03	1.50E-03	6.80E-04	5.98E-04	8.41E-04	5.83E-05
12	-	1.78E-03	1.50E-03	7.70E-04	5.51E-04	8.77E-04	6.89E-05
13	-	1.93E-03	1.50E-03	8.62E-04	5.09E-04	9.08E-04	7.98E-05
14	-	2.21E-03	1.50E-03	1.05E-03	4.39E-04	9.56E-04	1.02E-04
15	-	2.48E-03	1.50E-03	1.25E-03	3.83E-04	9.88E-04	1.25E-04
16	-	3.00E-03	1.50E-03	1.64E-03	3.02E-04	1.02E-03	1.71E-04
17	-	3.49E-03	1.50E-03	2.02E-03	2.48E-04	1.04E-03	2.14E-04

18	-	5.50E-03	1.50E-03	3.75E-03	1.27E-04	9.91E-04	3.79E-04
19	-	7.03E-03	1.50E-03	5.13E-03	8.71E-05	9.26E-04	4.84E-04
20	-	8.22E-03	1.50E-03	6.24E-03	6.77E-05	8.74E-04	5.56E-04

Measured chemical shifts

Point	pH	D1	D2
1	-	9.05E+00	8.47E+00
2	-	9.06E+00	8.48E+00
3	-	9.06E+00	8.49E+00
4	-	9.07E+00	8.50E+00
5	-	9.07E+00	8.51E+00
6	-	9.07E+00	8.52E+00
7	-	9.08E+00	8.53E+00
8	-	9.08E+00	8.54E+00
9	-	9.09E+00	8.55E+00
10	-	9.09E+00	8.56E+00
11	-	9.09E+00	8.56E+00
12	-	9.10E+00	8.57E+00
13	-	9.10E+00	8.57E+00
14	-	9.10E+00	8.58E+00
15	-	9.11E+00	8.59E+00
16	-	9.11E+00	8.60E+00
17	-	9.12E+00	8.61E+00
18	-	9.14E+00	8.63E+00
19	-	9.15E+00	8.64E+00
20	-	9.16E+00	8.64E+00

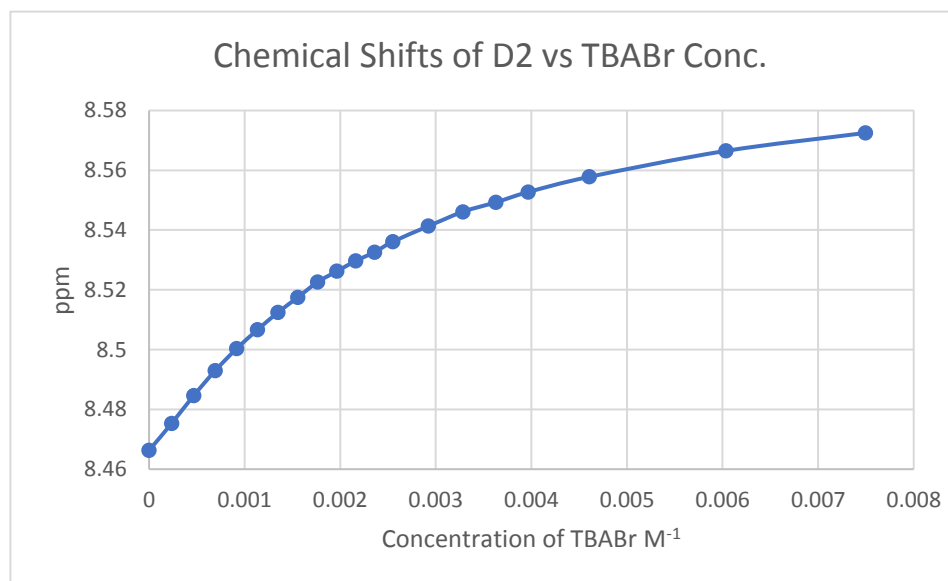
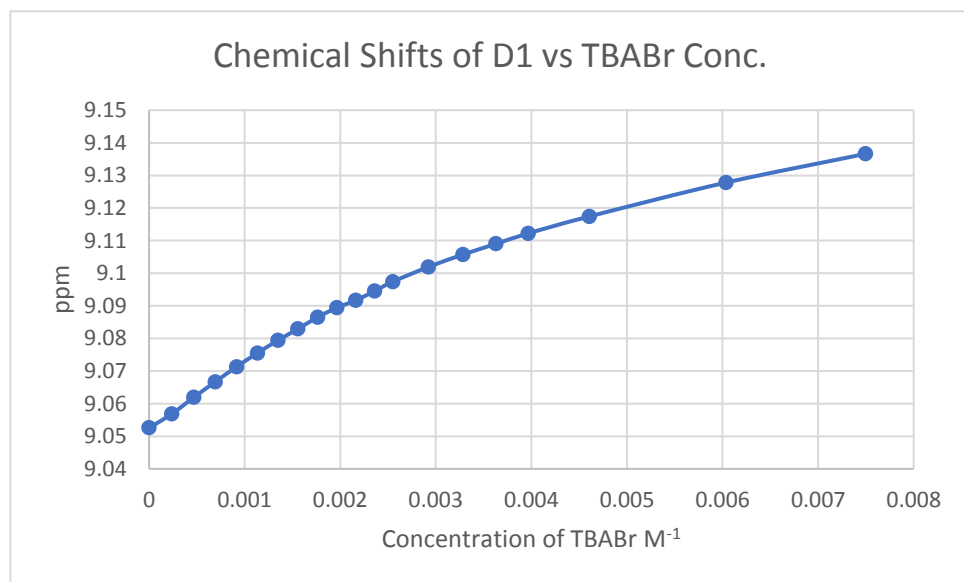
Calculated chemical shifts

Point	pH	D1	D2
1	-	9.05E+00	8.46E+00
2	-	9.06E+00	8.48E+00
3	-	9.06E+00	8.49E+00
4	-	9.07E+00	8.50E+00
5	-	9.07E+00	8.51E+00
6	-	9.07E+00	8.52E+00
7	-	9.08E+00	8.53E+00
8	-	9.08E+00	8.54E+00
9	-	9.09E+00	8.55E+00
10	-	9.09E+00	8.56E+00
11	-	9.09E+00	8.56E+00
12	-	9.09E+00	8.57E+00
13	-	9.10E+00	8.57E+00
14	-	9.10E+00	8.58E+00
15	-	9.11E+00	8.59E+00

16	-	9.11E+00	8.60E+00
17	-	9.12E+00	8.61E+00
18	-	9.14E+00	8.63E+00
19	-	9.15E+00	8.64E+00
20	-	9.16E+00	8.64E+00

Chemical shifts for each nucleus

species	D1	D2
H	9.05E+00	8.46E+00
GH	9.11E+00	8.62E+00
G ₂ H	9.26E+00	8.69E+00



G2HB and TBA⁺Br⁻ (Experiment 2)

Species	Log beta	G	H	std. dev.
				0.0817
1	3.3606	1	1	
2	5.5249	2	1	0.1511

Converged in 1 iterations with sigma = 0.797377

Species concentrations/mol dm⁻³

Point	pH	T(TBABr)	T(G2HB)	F(TBABr)	F(G2HB)	species 1	species 2
1	-	0.00E+00	1.49E-03	1.05E-90	1.49E-03	3.58E-90	5.49E-178
2	-	2.37E-04	1.49E-03	5.85E-05	1.31E-03	1.76E-04	1.50E-06
3	-	4.70E-04	1.49E-03	1.26E-04	1.15E-03	3.32E-04	6.10E-06
4	-	6.98E-04	1.49E-03	2.03E-04	1.01E-03	4.68E-04	1.38E-05
5	-	9.22E-04	1.49E-03	2.89E-04	8.80E-04	5.84E-04	2.46E-05
6	-	1.14E-03	1.49E-03	3.85E-04	7.70E-04	6.80E-04	3.82E-05
7	-	1.36E-03	1.49E-03	4.90E-04	6.76E-04	7.59E-04	5.42E-05
8	-	1.57E-03	1.49E-03	6.02E-04	5.95E-04	8.22E-04	7.22E-05
9	-	1.78E-03	1.49E-03	7.21E-04	5.26E-04	8.71E-04	9.17E-05
10	-	1.98E-03	1.49E-03	8.46E-04	4.68E-04	9.08E-04	1.12E-04
11	-	2.18E-03	1.49E-03	9.76E-04	4.19E-04	9.37E-04	1.33E-04
12	-	2.38E-03	1.49E-03	1.11E-03	3.76E-04	9.57E-04	1.55E-04
13	-	2.57E-03	1.49E-03	1.24E-03	3.41E-04	9.72E-04	1.76E-04
14	-	2.94E-03	1.49E-03	1.52E-03	2.83E-04	9.87E-04	2.19E-04
15	-	3.31E-03	1.49E-03	1.80E-03	2.40E-04	9.89E-04	2.60E-04
16	-	3.66E-03	1.49E-03	2.08E-03	2.07E-04	9.84E-04	2.98E-04
17	-	4.00E-03	1.49E-03	2.35E-03	1.80E-04	9.74E-04	3.34E-04
18	-	4.64E-03	1.49E-03	2.89E-03	1.43E-04	9.46E-04	4.00E-04
19	-	6.08E-03	1.49E-03	4.16E-03	9.12E-05	8.70E-04	5.28E-04
20	-	7.55E-03	1.49E-03	5.49E-03	6.28E-05	7.91E-04	6.34E-04

Measured chemical shifts

Point	pH	D1	D2
1	-	9.05E+00	8.46E+00
2	-	9.06E+00	8.48E+00
3	-	9.06E+00	8.50E+00
4	-	9.07E+00	8.51E+00
5	-	9.07E+00	8.53E+00
6	-	9.08E+00	8.54E+00
7	-	9.08E+00	8.55E+00

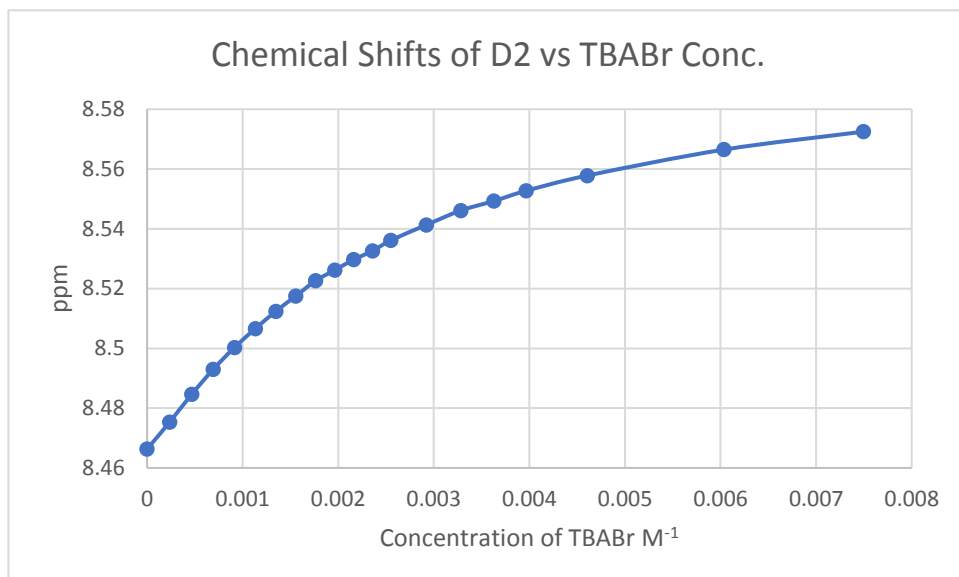
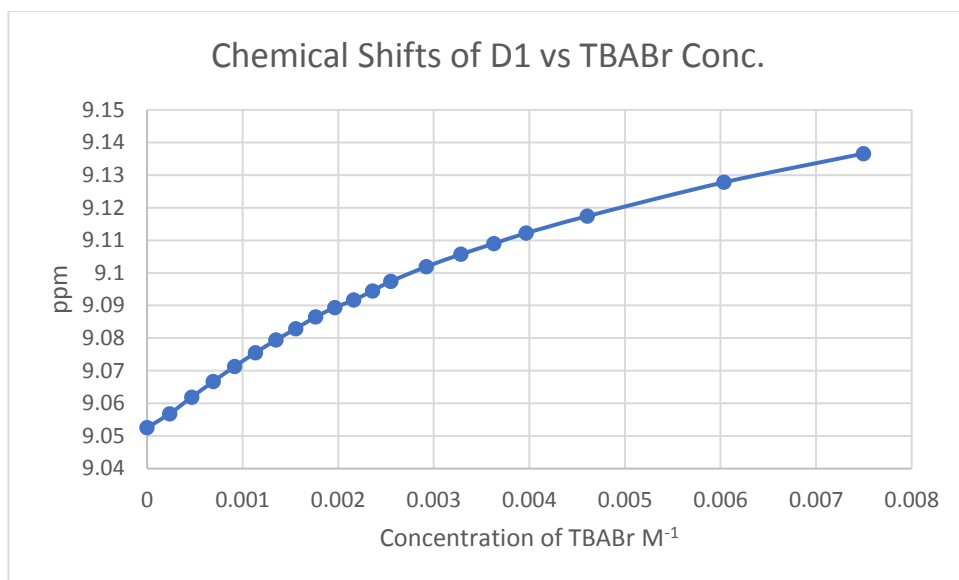
8	-	9.09E+00	8.56E+00
9	-	9.09E+00	8.57E+00
10	-	9.10E+00	8.58E+00
11	-	9.10E+00	8.58E+00
12	-	9.10E+00	8.59E+00
13	-	9.11E+00	8.59E+00
14	-	9.11E+00	8.60E+00
15	-	9.12E+00	8.61E+00
16	-	9.12E+00	8.61E+00
17	-	9.12E+00	8.62E+00
18	-	9.13E+00	8.62E+00
19	-	9.14E+00	8.63E+00
20	-	9.16E+00	8.64E+00

Calculated chemical shifts

Point	pH	D1	D2
1	-	9.05E+00	8.46E+00
2	-	9.06E+00	8.48E+00
3	-	9.06E+00	8.50E+00
4	-	9.07E+00	8.51E+00
5	-	9.07E+00	8.53E+00
6	-	9.08E+00	8.54E+00
7	-	9.08E+00	8.55E+00
8	-	9.09E+00	8.56E+00
9	-	9.09E+00	8.57E+00
10	-	9.10E+00	8.58E+00
11	-	9.10E+00	8.58E+00
12	-	9.10E+00	8.59E+00
13	-	9.11E+00	8.59E+00
14	-	9.11E+00	8.60E+00
15	-	9.12E+00	8.61E+00
16	-	9.12E+00	8.61E+00
17	-	9.13E+00	8.62E+00
18	-	9.13E+00	8.62E+00
19	-	9.15E+00	8.63E+00
20	-	9.16E+00	8.64E+00

Chemical shifts for each nucleus

species	D1	D2	
H	9.05E+00	8.46E+00	0.00E+00
GH	9.10E+00	8.62E+00	0.00E+00
G ₂ H	9.23E+00	8.68E+00	0.00E+00



G2HB and TBA⁺Br⁻ (Experiment 3)

Species	Log beta	G	H	std. dev.
1	3.2951	1	1	0.099
2	5.4954	2	1	0.1711

Converged in 1 iterations with sigma = 0.865558

Species concentrations/mol dm⁻³

Point	pH	T(TBABr)	T(G2HB)	F(TBABr)	F(G2HB)	species 1	species 2
1	-	0.00E+00	1.49E-03	1.13E-90	1.49E-03	3.32E-90	5.96E-178
2	-	2.37E-04	1.49E-03	6.50E-05	1.32E-03	1.69E-04	1.74E-06

3	-	4.70E-04	1.49E-03	1.38E-04	1.16E-03	3.18E-04	6.97E-06
4	-	6.98E-04	1.49E-03	2.20E-04	1.03E-03	4.46E-04	1.56E-05
5	-	9.22E-04	1.49E-03	3.11E-04	9.05E-04	5.56E-04	2.74E-05
6	-	1.14E-03	1.49E-03	4.10E-04	8.00E-04	6.47E-04	4.21E-05
7	-	1.36E-03	1.49E-03	5.17E-04	7.08E-04	7.22E-04	5.92E-05
8	-	1.57E-03	1.49E-03	6.30E-04	6.29E-04	7.82E-04	7.81E-05
9	-	1.78E-03	1.49E-03	7.49E-04	5.61E-04	8.29E-04	9.85E-05
10	-	1.98E-03	1.49E-03	8.73E-04	5.03E-04	8.66E-04	1.20E-04
11	-	2.18E-03	1.49E-03	1.00E-03	4.53E-04	8.94E-04	1.42E-04
12	-	2.38E-03	1.49E-03	1.13E-03	4.10E-04	9.15E-04	1.64E-04
13	-	2.57E-03	1.49E-03	1.27E-03	3.72E-04	9.30E-04	1.87E-04
14	-	2.94E-03	1.49E-03	1.54E-03	3.12E-04	9.46E-04	2.31E-04
15	-	3.31E-03	1.49E-03	1.81E-03	2.66E-04	9.50E-04	2.73E-04
16	-	3.66E-03	1.49E-03	2.09E-03	2.30E-04	9.46E-04	3.13E-04
17	-	4.00E-03	1.49E-03	2.36E-03	2.01E-04	9.37E-04	3.50E-04
18	-	4.64E-03	1.49E-03	2.89E-03	1.60E-04	9.11E-04	4.18E-04
19	-	6.08E-03	1.49E-03	4.15E-03	1.02E-04	8.36E-04	5.50E-04
20	-	7.55E-03	1.49E-03	5.47E-03	7.03E-05	7.59E-04	6.59E-04

Measured chemical shifts

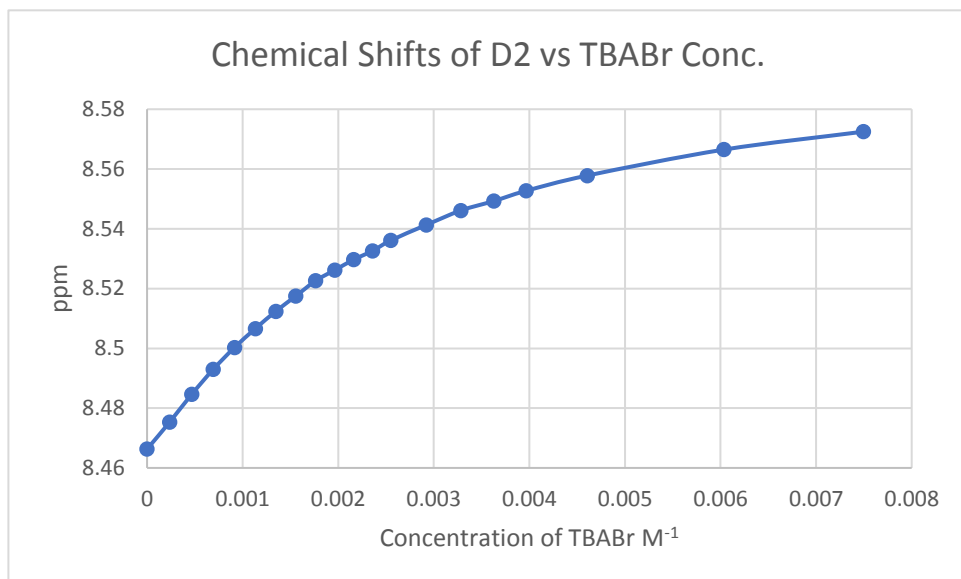
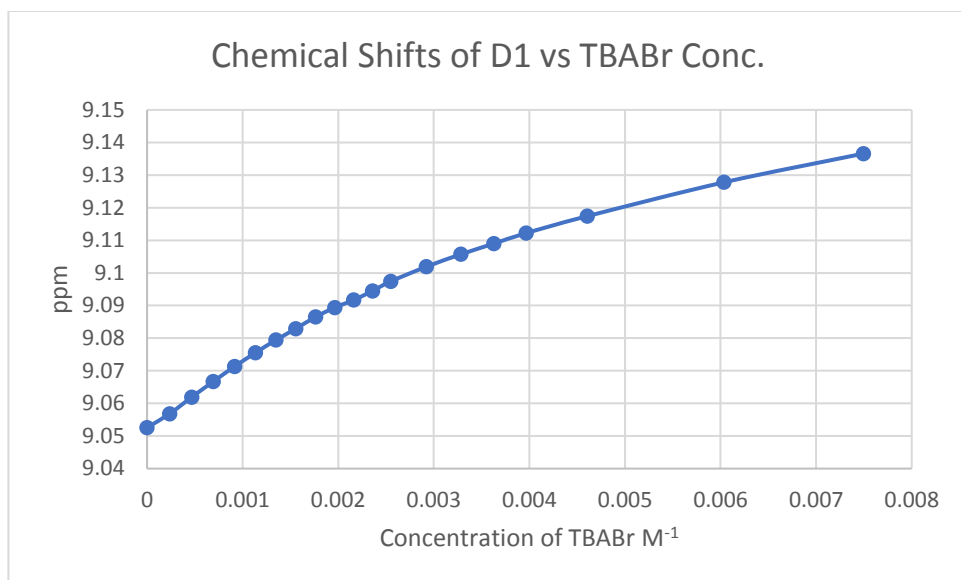
Point	pH	D1	D2
1	-	9.05E+00	8.47E+00
2	-	9.06E+00	8.48E+00
3	-	9.06E+00	8.50E+00
4	-	9.07E+00	8.51E+00
5	-	9.07E+00	8.52E+00
6	-	9.08E+00	8.54E+00
7	-	9.08E+00	8.55E+00
8	-	9.09E+00	8.56E+00
9	-	9.09E+00	8.56E+00
10	-	9.10E+00	8.57E+00
11	-	9.10E+00	8.58E+00
12	-	9.10E+00	8.58E+00
13	-	9.11E+00	8.59E+00
14	-	9.11E+00	8.60E+00
15	-	9.12E+00	8.60E+00
16	-	9.12E+00	8.61E+00
17	-	9.12E+00	8.61E+00
18	-	9.13E+00	8.62E+00
19	-	9.14E+00	8.63E+00
20	-	9.16E+00	8.64E+00

Calculated chemical shifts

Point	pH	D1	D2
1	-	9.05E+00	8.46E+00
2	-	9.06E+00	8.48E+00
3	-	9.06E+00	8.50E+00
4	-	9.07E+00	8.51E+00
5	-	9.07E+00	8.53E+00
6	-	9.08E+00	8.54E+00
7	-	9.08E+00	8.55E+00
8	-	9.09E+00	8.56E+00
9	-	9.09E+00	8.56E+00
10	-	9.10E+00	8.57E+00
11	-	9.10E+00	8.58E+00
12	-	9.10E+00	8.58E+00
13	-	9.11E+00	8.59E+00
14	-	9.11E+00	8.60E+00
15	-	9.12E+00	8.60E+00
16	-	9.12E+00	8.61E+00
17	-	9.12E+00	8.61E+00
18	-	9.13E+00	8.62E+00
19	-	9.14E+00	8.63E+00
20	-	9.15E+00	8.64E+00

Chemical shifts for each nucleus

species	D1	D2
H	9.05E+00	8.46E+00
GH	9.10E+00	8.62E+00
G ₂ H	9.22E+00	8.68E+00



G2HB and TBA⁺I⁻ (Experiment 1)

Species	Log beta	G	H	std. dev.
1	3.1577	1	1	0.1384
2	5.1428	2	1	0.2601

Converged in 1 iterations with sigma = 0.050258

Species concentrations/mol dm⁻³

Point	pH	T(TBAI)	T(G2HB)	F(TBAI)	F(G2HB)	species 1	species 2
1	-	0.00E+00	1.46E-03	1.29E-90	1.46E-03	2.70E-90	3.37E-178
2	-	1.64E-04	1.46E-03	5.55E-05	1.35E-03	1.08E-04	5.77E-07
3	-	3.25E-04	1.46E-03	1.15E-04	1.25E-03	2.06E-04	2.28E-06
4	-	4.83E-04	1.46E-03	1.78E-04	1.16E-03	2.96E-04	5.07E-06

5	-	6.38E-04	1.46E-03	2.44E-04	1.07E-03	3.76E-04	8.88E-06
6	-	7.90E-04	1.46E-03	3.14E-04	9.95E-04	4.49E-04	1.36E-05
7	-	9.39E-04	1.46E-03	3.87E-04	9.24E-04	5.14E-04	1.92E-05
8	-	1.09E-03	1.46E-03	4.62E-04	8.60E-04	5.72E-04	2.56E-05
9	-	1.23E-03	1.46E-03	5.41E-04	8.02E-04	6.23E-04	3.26E-05
10	-	1.37E-03	1.46E-03	6.21E-04	7.49E-04	6.69E-04	4.01E-05
11	-	1.51E-03	1.46E-03	7.03E-04	7.01E-04	7.09E-04	4.82E-05
12	-	1.64E-03	1.46E-03	7.87E-04	6.57E-04	7.44E-04	5.66E-05
13	-	1.78E-03	1.46E-03	8.72E-04	6.18E-04	7.75E-04	6.53E-05
14	-	2.04E-03	1.46E-03	1.05E-03	5.49E-04	8.25E-04	8.34E-05
15	-	2.29E-03	1.46E-03	1.22E-03	4.92E-04	8.64E-04	1.02E-04
16	-	2.77E-03	1.46E-03	1.57E-03	4.04E-04	9.14E-04	1.39E-04
17	-	3.21E-03	1.46E-03	1.92E-03	3.41E-04	9.42E-04	1.75E-04
18	-	5.07E-03	1.46E-03	3.48E-03	1.90E-04	9.49E-04	3.19E-04
19	-	6.48E-03	1.46E-03	4.74E-03	1.33E-04	9.09E-04	4.16E-04
20	-	7.58E-03	1.46E-03	5.74E-03	1.05E-04	8.70E-04	4.82E-04

Measured chemical shifts

Point	pH	D1	D2
1	-	9.05E+00	8.47E+00
2	-	9.05E+00	8.47E+00
3	-	9.06E+00	8.48E+00
4	-	9.06E+00	8.49E+00
5	-	9.07E+00	8.49E+00
6	-	9.07E+00	8.50E+00
7	-	9.07E+00	8.50E+00
8	-	9.07E+00	8.51E+00
9	-	9.08E+00	8.51E+00
10	-	9.08E+00	8.51E+00
11	-	9.08E+00	8.52E+00
12	-	9.08E+00	8.52E+00
13	-	9.09E+00	8.52E+00
14	-	9.09E+00	8.53E+00
15	-	9.09E+00	8.53E+00
16	-	9.10E+00	8.54E+00
17	-	9.10E+00	8.54E+00
18	-	9.12E+00	8.56E+00
19	-	9.13E+00	8.57E+00
20	-	9.14E+00	8.57E+00

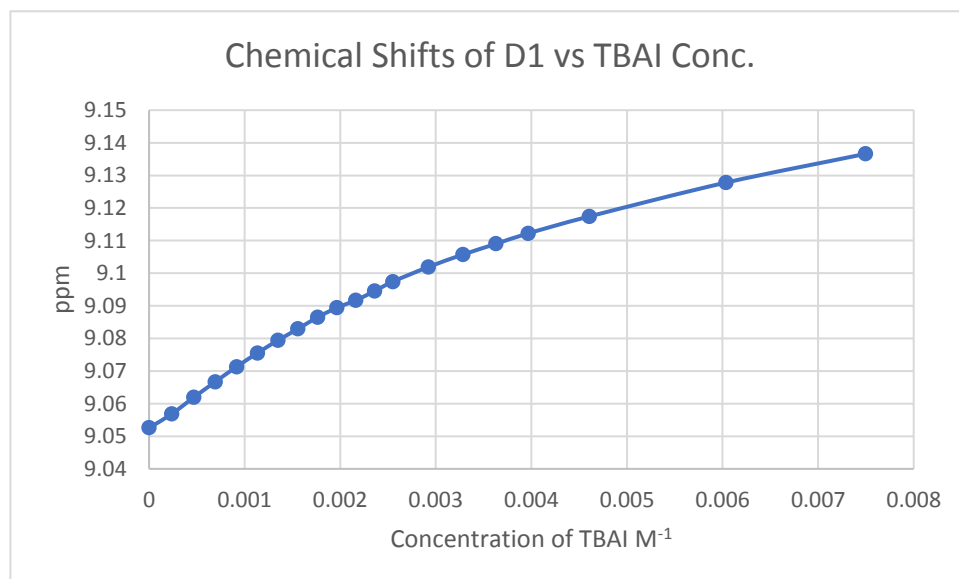
Calculated chemical shifts

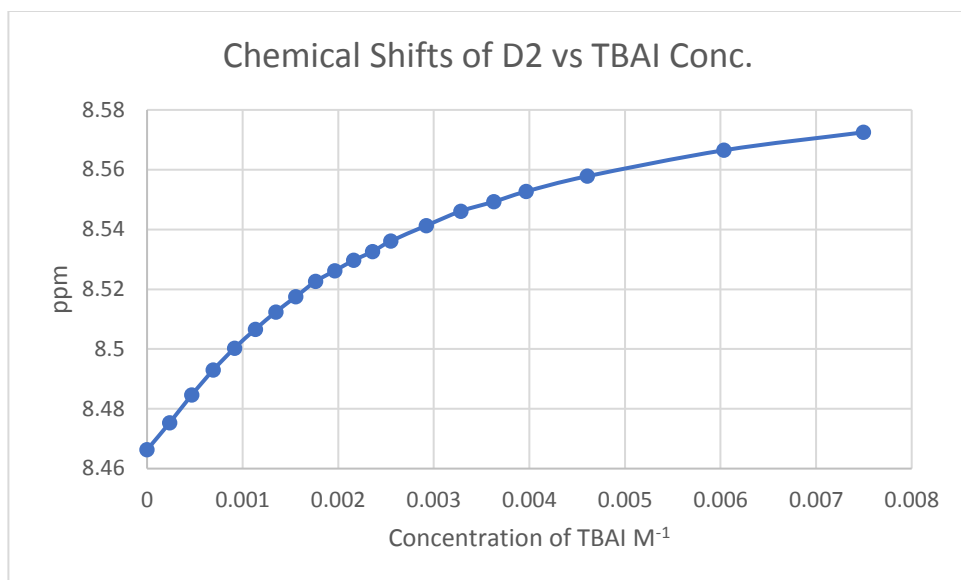
Point	pH	D1	D2
1	-	9.05E+00	8.47E+00
2	-	9.06E+00	8.47E+00

3	-	9.06E+00	8.48E+00
4	-	9.06E+00	8.49E+00
5	-	9.07E+00	8.49E+00
6	-	9.07E+00	8.50E+00
7	-	9.07E+00	8.50E+00
8	-	9.07E+00	8.51E+00
9	-	9.08E+00	8.51E+00
10	-	9.08E+00	8.51E+00
11	-	9.08E+00	8.52E+00
12	-	9.08E+00	8.52E+00
13	-	9.09E+00	8.52E+00
14	-	9.09E+00	8.53E+00
15	-	9.09E+00	8.53E+00
16	-	9.10E+00	8.54E+00
17	-	9.10E+00	8.54E+00
18	-	9.12E+00	8.56E+00
19	-	9.13E+00	8.57E+00
20	-	9.14E+00	8.57E+00

Chemical shifts for each nucleus

species	D1	D2
H	9.05E+00	8.47E+00
GH	9.10E+00	8.56E+00
G ₂ H	9.21E+00	8.62E+00





G2HB and TBAI⁺I⁻ (Experiment 2)

Species	Log beta	G	H	std. dev.
1	3.2155	1	1	0.0788
2	5.2713	2	1	0.1354

Converged in 1 iterations with sigma = 0.325618

Species concentrations/mol dm⁻³

Point	pH	T(TBAI)	T(G2HB)	F(TBAI)	F(G2HB)	species 1	species 2
1	-	0.00E+00	1.52E-03	1.24E-90	1.52E-03	3.09E-90	4.37E-178
2	-	2.36E-04	1.52E-03	7.23E-05	1.35E-03	1.61E-04	1.32E-06
3	-	4.67E-04	1.52E-03	1.53E-04	1.21E-03	3.03E-04	5.27E-06
4	-	6.93E-04	1.52E-03	2.42E-04	1.08E-03	4.28E-04	1.18E-05
5	-	9.15E-04	1.52E-03	3.39E-04	9.60E-04	5.35E-04	2.06E-05
6	-	1.13E-03	1.52E-03	4.44E-04	8.58E-04	6.26E-04	3.16E-05
7	-	1.35E-03	1.52E-03	5.56E-04	7.69E-04	7.02E-04	4.44E-05
8	-	1.56E-03	1.52E-03	6.74E-04	6.91E-04	7.65E-04	5.86E-05
9	-	1.76E-03	1.52E-03	7.97E-04	6.24E-04	8.17E-04	7.41E-05
10	-	1.96E-03	1.52E-03	9.25E-04	5.66E-04	8.59E-04	9.03E-05
11	-	2.16E-03	1.52E-03	1.06E-03	5.15E-04	8.93E-04	1.07E-04
12	-	2.36E-03	1.52E-03	1.19E-03	4.71E-04	9.20E-04	1.24E-04
13	-	2.55E-03	1.52E-03	1.32E-03	4.32E-04	9.41E-04	1.42E-04
14	-	2.92E-03	1.52E-03	1.60E-03	3.69E-04	9.70E-04	1.76E-04
15	-	3.28E-03	1.52E-03	1.88E-03	3.20E-04	9.85E-04	2.10E-04
16	-	3.63E-03	1.52E-03	2.15E-03	2.81E-04	9.92E-04	2.43E-04

17	-	3.97E-03	1.52E-03	2.43E-03	2.49E-04	9.92E-04	2.74E-04
18	-	4.60E-03	1.52E-03	2.96E-03	2.02E-04	9.82E-04	3.31E-04
19	-	6.04E-03	1.52E-03	4.21E-03	1.35E-04	9.33E-04	4.47E-04
20	-	7.50E-03	1.52E-03	5.53E-03	9.60E-05	8.71E-04	5.48E-04

Measured chemical shifts

Point	pH	D1	D2
1	-	9.05E+00	8.47E+00
2	-	9.06E+00	8.48E+00
3	-	9.06E+00	8.48E+00
4	-	9.07E+00	8.49E+00
5	-	9.07E+00	8.50E+00
6	-	9.08E+00	8.51E+00
7	-	9.08E+00	8.51E+00
8	-	9.08E+00	8.52E+00
9	-	9.09E+00	8.52E+00
10	-	9.09E+00	8.53E+00
11	-	9.09E+00	8.53E+00
12	-	9.09E+00	8.53E+00
13	-	9.10E+00	8.54E+00
14	-	9.10E+00	8.54E+00
15	-	9.11E+00	8.55E+00
16	-	9.11E+00	8.55E+00
17	-	9.11E+00	8.55E+00
18	-	9.12E+00	8.56E+00
19	-	9.13E+00	8.57E+00
20	-	9.14E+00	8.57E+00

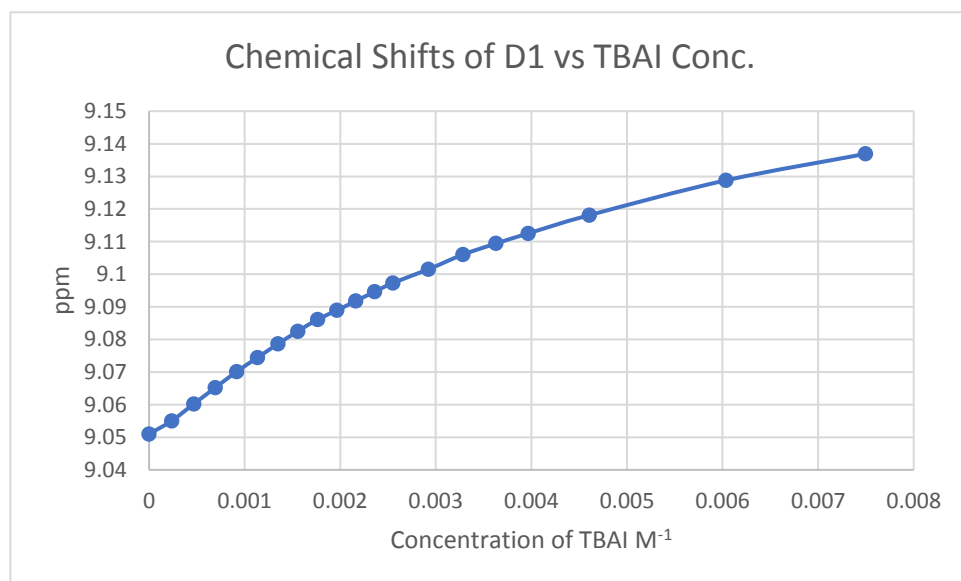
Calculated chemical shifts

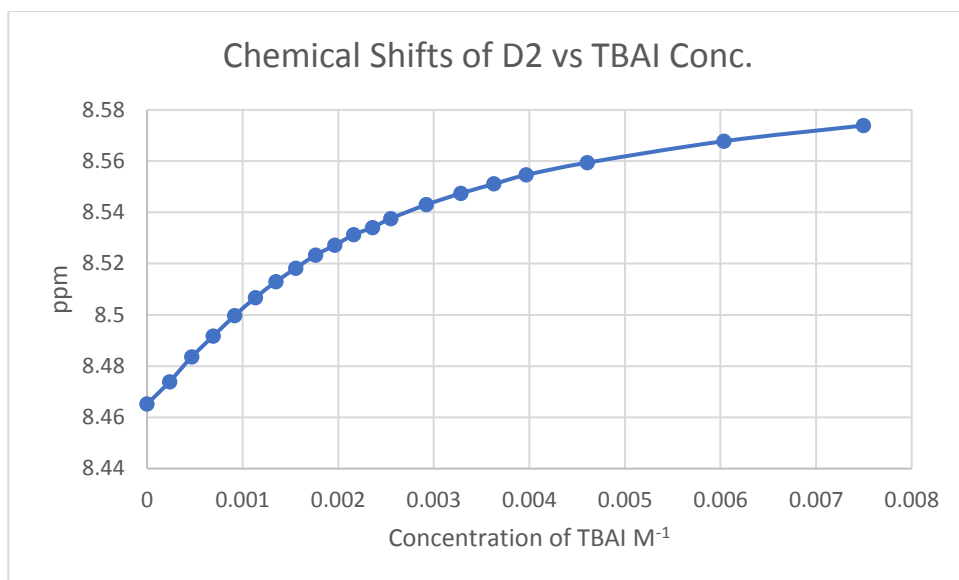
Point	pH	D1	D2
1	-	9.05E+00	8.47E+00
2	-	9.06E+00	8.48E+00
3	-	9.06E+00	8.48E+00
4	-	9.07E+00	8.49E+00
5	-	9.07E+00	8.50E+00
6	-	9.08E+00	8.51E+00
7	-	9.08E+00	8.51E+00
8	-	9.08E+00	8.52E+00
9	-	9.09E+00	8.52E+00
10	-	9.09E+00	8.53E+00
11	-	9.09E+00	8.53E+00
12	-	9.09E+00	8.53E+00
13	-	9.10E+00	8.54E+00

14	-	9.10E+00	8.54E+00
15	-	9.11E+00	8.55E+00
16	-	9.11E+00	8.55E+00
17	-	9.11E+00	8.55E+00
18	-	9.12E+00	8.56E+00
19	-	9.13E+00	8.57E+00
20	-	9.14E+00	8.57E+00

Chemical shifts for each nucleus

species	D1	D2
H	9.05E+00	8.47E+00
GH	9.10E+00	8.56E+00
G ₂ H	9.21E+00	8.62E+00





G2HB and TBAI⁺ (Experiment 3)

Species	Log beta	G	H	std. dev.
1	3.3579	1	1	0.0889
2	5.5695	2	1	0.1277

Converged in 1 iterations with sigma = 0.370939

Species concentrations/mol dm⁻³

Point	pH	T(TBAI)	T(G2HB)	F(TBAI)	F(G2HB)	species 1	species 2
1	-	0.00E+00	1.52E-03	1.06E-90	1.52E-03	3.67E-90	6.35E-178
2	-	2.36E-04	1.52E-03	5.73E-05	1.34E-03	1.75E-04	1.63E-06
3	-	4.67E-04	1.52E-03	1.23E-04	1.18E-03	3.30E-04	6.61E-06
4	-	6.93E-04	1.52E-03	1.97E-04	1.03E-03	4.66E-04	1.50E-05
5	-	9.15E-04	1.52E-03	2.81E-04	9.08E-04	5.81E-04	2.66E-05
6	-	1.13E-03	1.52E-03	3.73E-04	7.97E-04	6.78E-04	4.12E-05
7	-	1.35E-03	1.52E-03	4.74E-04	7.01E-04	7.56E-04	5.83E-05
8	-	1.56E-03	1.52E-03	5.82E-04	6.18E-04	8.20E-04	7.76E-05
9	-	1.76E-03	1.52E-03	6.96E-04	5.48E-04	8.69E-04	9.85E-05
10	-	1.96E-03	1.52E-03	8.16E-04	4.88E-04	9.07E-04	1.21E-04
11	-	2.16E-03	1.52E-03	9.41E-04	4.36E-04	9.36E-04	1.43E-04
12	-	2.36E-03	1.52E-03	1.07E-03	3.93E-04	9.56E-04	1.66E-04
13	-	2.55E-03	1.52E-03	1.20E-03	3.55E-04	9.71E-04	1.90E-04
14	-	2.92E-03	1.52E-03	1.47E-03	2.95E-04	9.85E-04	2.35E-04
15	-	3.28E-03	1.52E-03	1.74E-03	2.49E-04	9.87E-04	2.79E-04
16	-	3.63E-03	1.52E-03	2.01E-03	2.14E-04	9.80E-04	3.20E-04
17	-	3.97E-03	1.52E-03	2.28E-03	1.87E-04	9.69E-04	3.59E-04
18	-	4.60E-03	1.52E-03	2.81E-03	1.47E-04	9.39E-04	4.29E-04
19	-	6.04E-03	1.52E-03	4.05E-03	9.29E-05	8.57E-04	5.65E-04
20	-	7.50E-03	1.52E-03	5.37E-03	6.33E-05	7.75E-04	6.77E-04

Measured chemical shifts

Point	pH	D1	D2
1	-	9.05E+00	8.47E+00
2	-	9.06E+00	8.47E+00
3	-	9.06E+00	8.48E+00
4	-	9.07E+00	8.49E+00
5	-	9.07E+00	8.50E+00
6	-	9.07E+00	8.51E+00
7	-	9.08E+00	8.51E+00
8	-	9.08E+00	8.52E+00
9	-	9.09E+00	8.52E+00
10	-	9.09E+00	8.53E+00
11	-	9.09E+00	8.53E+00
12	-	9.09E+00	8.53E+00
13	-	9.10E+00	8.54E+00
14	-	9.10E+00	8.54E+00
15	-	9.11E+00	8.55E+00
16	-	9.11E+00	8.55E+00
17	-	9.11E+00	8.55E+00
18	-	9.12E+00	8.56E+00
19	-	9.13E+00	8.57E+00
20	-	9.14E+00	8.57E+00

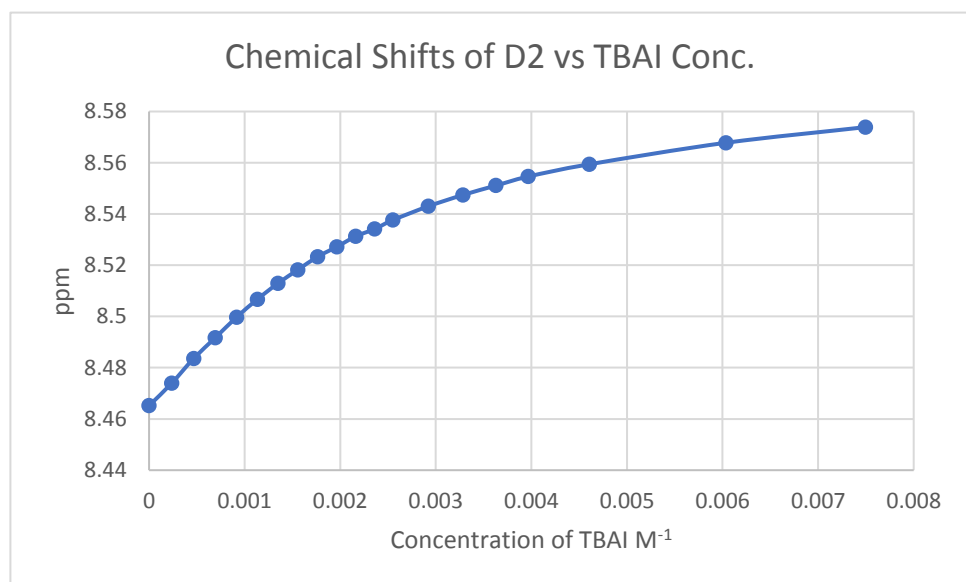
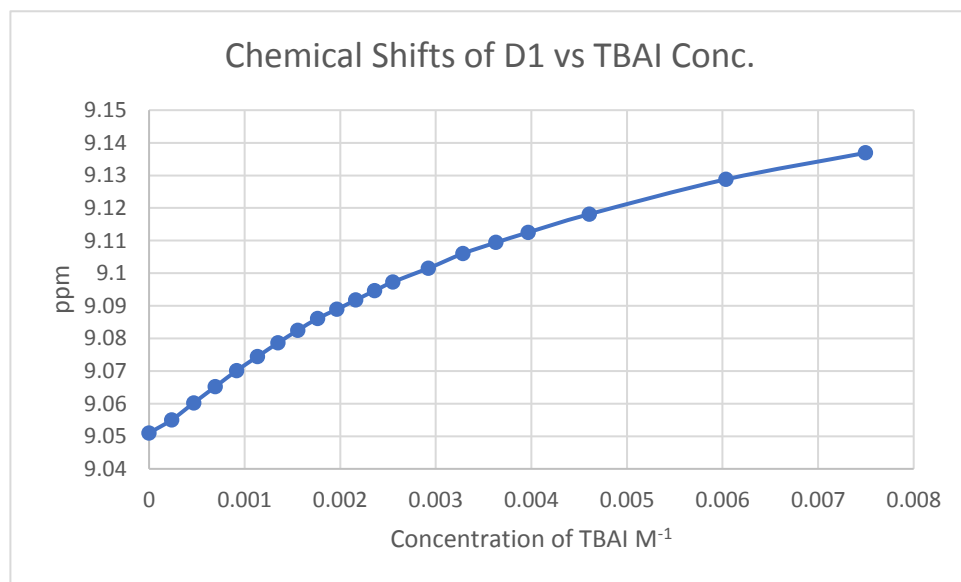
Calculated chemical shifts

Point	pH	D1	D2
1	-	9.05E+00	8.46E+00
2	-	9.06E+00	8.47E+00
3	-	9.06E+00	8.48E+00
4	-	9.07E+00	8.49E+00
5	-	9.07E+00	8.50E+00
6	-	9.07E+00	8.51E+00
7	-	9.08E+00	8.51E+00
8	-	9.08E+00	8.52E+00
9	-	9.09E+00	8.52E+00
10	-	9.09E+00	8.53E+00
11	-	9.09E+00	8.53E+00
12	-	9.09E+00	8.53E+00
13	-	9.10E+00	8.54E+00
14	-	9.10E+00	8.54E+00
15	-	9.11E+00	8.55E+00
16	-	9.11E+00	8.55E+00
17	-	9.11E+00	8.55E+00

18	-	9.12E+00	8.56E+00
19	-	9.13E+00	8.57E+00
20	-	9.14E+00	8.57E+00

Chemical shifts for each nucleus

species	D1	D2
H	9.05E+00	8.46E+00
GH	9.10E+00	8.55E+00
G ₂ H	9.19E+00	8.61E+00



G1HB and TBA⁺Cl⁻ (Experiment 1)

Species	Log beta	G	H	std. dev.
1	3.943	1	1	0.6552
2	6.3542	2	1	0.6534

Converged in 1 iterations with sigma = 0.151280

Species concentrations/mol dm⁻³

Point	pH	T(TBACl)	T(G1HB)	F(TBACl)	F(G1HB)	species 1	species 2
1	-	0.00E+00	1.56E-03	4.92E-91	1.56E-03	6.73E-90	8.53E-178
2	-	1.72E-04	1.56E-03	1.29E-05	1.40E-03	1.58E-04	5.27E-07
3	-	3.41E-04	1.56E-03	2.82E-05	1.25E-03	3.09E-04	2.24E-06
4	-	5.07E-04	1.56E-03	4.65E-05	1.10E-03	4.50E-04	5.39E-06
5	-	6.70E-04	1.56E-03	6.84E-05	9.68E-04	5.81E-04	1.02E-05
6	-	8.29E-04	1.56E-03	9.48E-05	8.42E-04	7.00E-04	1.71E-05
7	-	9.86E-04	1.56E-03	1.27E-04	7.27E-04	8.06E-04	2.63E-05
8	-	1.14E-03	1.56E-03	1.64E-04	6.23E-04	8.98E-04	3.81E-05
9	-	1.29E-03	1.56E-03	2.09E-04	5.31E-04	9.75E-04	5.26E-05
10	-	1.44E-03	1.56E-03	2.61E-04	4.53E-04	1.04E-03	6.98E-05
11	-	1.58E-03	1.56E-03	3.20E-04	3.86E-04	1.08E-03	8.94E-05
12	-	1.73E-03	1.56E-03	3.86E-04	3.31E-04	1.12E-03	1.11E-04
13	-	1.87E-03	1.56E-03	4.57E-04	2.85E-04	1.14E-03	1.34E-04
14	-	2.14E-03	1.56E-03	6.12E-04	2.16E-04	1.16E-03	1.83E-04
15	-	2.40E-03	1.56E-03	7.79E-04	1.69E-04	1.16E-03	2.32E-04
16	-	2.90E-03	1.56E-03	1.13E-03	1.13E-04	1.12E-03	3.26E-04
17	-	3.37E-03	1.56E-03	1.48E-03	8.21E-05	1.07E-03	4.09E-04
18	-	5.32E-03	1.56E-03	3.11E-03	3.11E-05	8.48E-04	6.80E-04
19	-	6.79E-03	1.56E-03	4.43E-03	1.85E-05	7.19E-04	8.22E-04
20	-	7.95E-03	1.56E-03	5.50E-03	1.33E-05	6.40E-04	9.06E-04

Measured chemical shifts

Point	pH	D1
1	-	9.08E+00
2	-	9.09E+00
3	-	9.10E+00
4	-	9.11E+00
5	-	9.11E+00
6	-	9.12E+00
7	-	9.13E+00
8	-	9.14E+00
9	-	9.15E+00
10	-	9.15E+00
11	-	9.16E+00
12	-	9.16E+00
13	-	9.17E+00

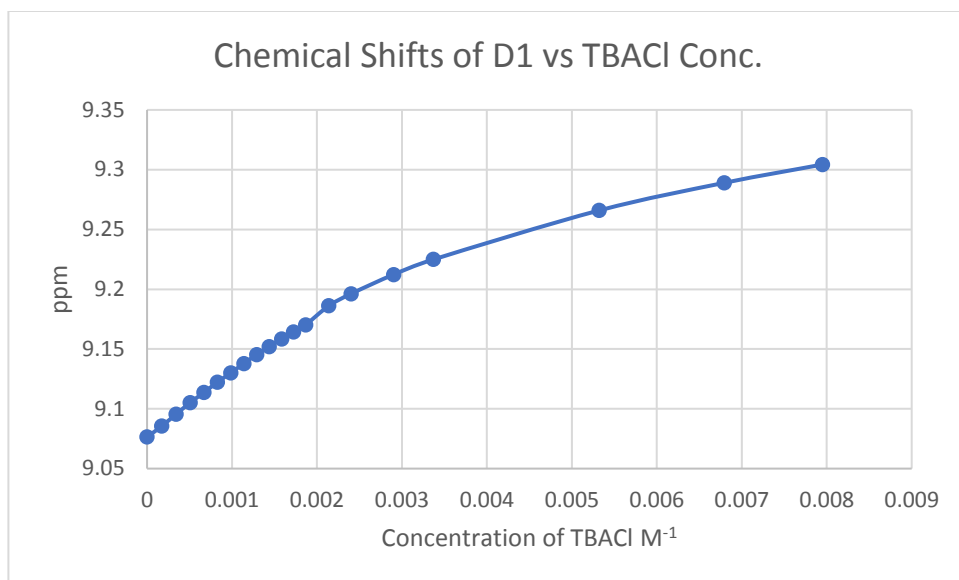
14	-	9.19E+00
15	-	9.20E+00
16	-	9.21E+00
17	-	9.22E+00
18	-	9.27E+00
19	-	9.29E+00
20	-	9.30E+00

Calculated chemical shifts

Point	pH	D1
1	-	9.08E+00
2	-	9.09E+00
3	-	9.10E+00
4	-	9.10E+00
5	-	9.11E+00
6	-	9.12E+00
7	-	9.13E+00
8	-	9.14E+00
9	-	9.15E+00
10	-	9.15E+00
11	-	9.16E+00
12	-	9.17E+00
13	-	9.17E+00
14	-	9.18E+00
15	-	9.19E+00
16	-	9.21E+00
17	-	9.23E+00
18	-	9.27E+00
19	-	9.29E+00
20	-	9.30E+00

Chemical shifts for each nucleus

species	D1
H	9.08E+00
GH	9.17E+00
G ₂ H	9.40E+00



G1HB and TBA⁺Cl⁻ (Experiment 2)

Species	Log beta	G	H	std. dev.
1	4.1021	1	1	0.0258
2	6.3622	2	1	0.0265

Converged in 1 iterations with sigma = 0.079732

Species concentrations/mol dm⁻³

Point	pH	T(TBACl)	T(G1HB)	F(TBACl)	F(G1HB)	species 1	species 2
1	-	0.00E+00	1.52E-03	4.13E-91	1.52E-03	7.95E-90	5.97E-178
2	-	2.66E-04	1.52E-03	1.55E-05	1.27E-03	2.49E-04	7.01E-07
3	-	5.26E-04	1.52E-03	3.69E-05	1.03E-03	4.83E-04	3.24E-06
4	-	7.82E-04	1.52E-03	6.76E-05	8.15E-04	6.97E-04	8.57E-06
5	-	1.03E-03	1.52E-03	1.13E-04	6.20E-04	8.83E-04	1.81E-05
6	-	1.28E-03	1.52E-03	1.79E-04	4.56E-04	1.03E-03	3.36E-05
7	-	1.52E-03	1.52E-03	2.72E-04	3.30E-04	1.13E-03	5.62E-05
8	-	1.76E-03	1.52E-03	3.91E-04	2.41E-04	1.19E-03	8.50E-05
9	-	1.99E-03	1.52E-03	5.31E-04	1.82E-04	1.22E-03	1.18E-04
10	-	2.22E-03	1.52E-03	6.84E-04	1.42E-04	1.23E-03	1.53E-04
11	-	2.66E-03	1.52E-03	1.01E-03	9.42E-05	1.20E-03	2.22E-04
12	-	3.09E-03	1.52E-03	1.35E-03	6.84E-05	1.17E-03	2.86E-04
13	-	3.50E-03	1.52E-03	1.69E-03	5.26E-05	1.12E-03	3.45E-04
14	-	3.90E-03	1.52E-03	2.02E-03	4.22E-05	1.08E-03	3.98E-04
15	-	4.28E-03	1.52E-03	2.35E-03	3.49E-05	1.04E-03	4.46E-04
16	-	4.66E-03	1.52E-03	2.68E-03	2.96E-05	1.00E-03	4.89E-04
17	-	5.02E-03	1.52E-03	2.99E-03	2.55E-05	9.68E-04	5.28E-04
18	-	5.37E-03	1.52E-03	3.31E-03	2.24E-05	9.36E-04	5.63E-04
19	-	6.35E-03	1.52E-03	4.19E-03	1.61E-05	8.53E-04	6.51E-04
20	-	7.53E-03	1.52E-03	5.28E-03	1.15E-05	7.70E-04	7.40E-04

Measured chemical shifts

Point	pH	D1	D2
1	-	8.52E+00	7.91E+00
2	-	8.53E+00	7.91E+00
3	-	8.54E+00	7.91E+00
4	-	8.55E+00	7.91E+00
5	-	8.57E+00	7.91E+00
6	-	8.58E+00	7.91E+00
7	-	8.59E+00	7.91E+00
8	-	8.60E+00	7.91E+00
9	-	8.61E+00	7.92E+00
10	-	8.61E+00	7.92E+00
11	-	8.63E+00	7.92E+00
12	-	8.64E+00	7.92E+00
13	-	8.65E+00	7.92E+00
14	-	8.66E+00	7.92E+00
15	-	8.67E+00	7.92E+00
16	-	8.68E+00	7.92E+00
17	-	8.68E+00	7.92E+00
18	-	8.69E+00	7.92E+00
19	-	8.70E+00	7.93E+00
20	-	8.72E+00	7.93E+00

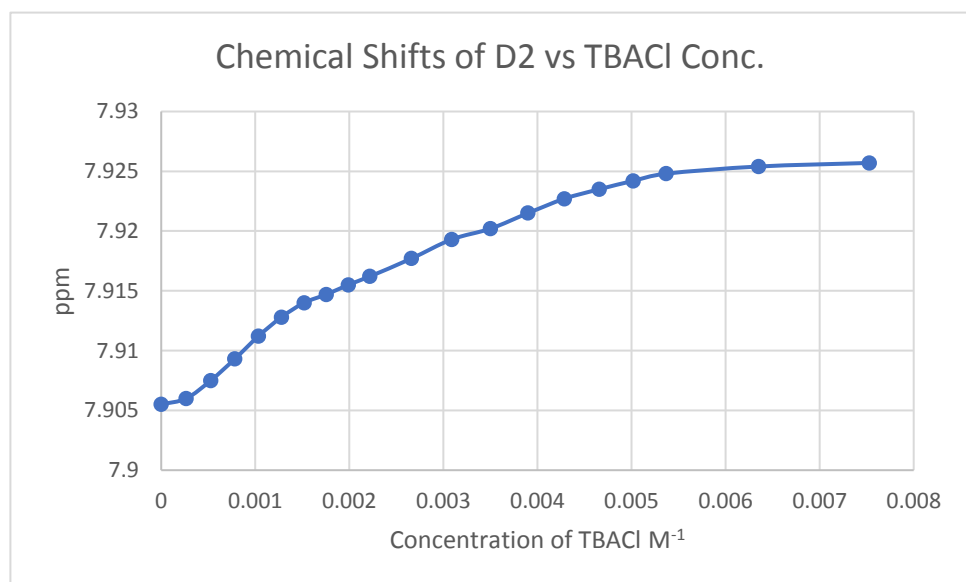
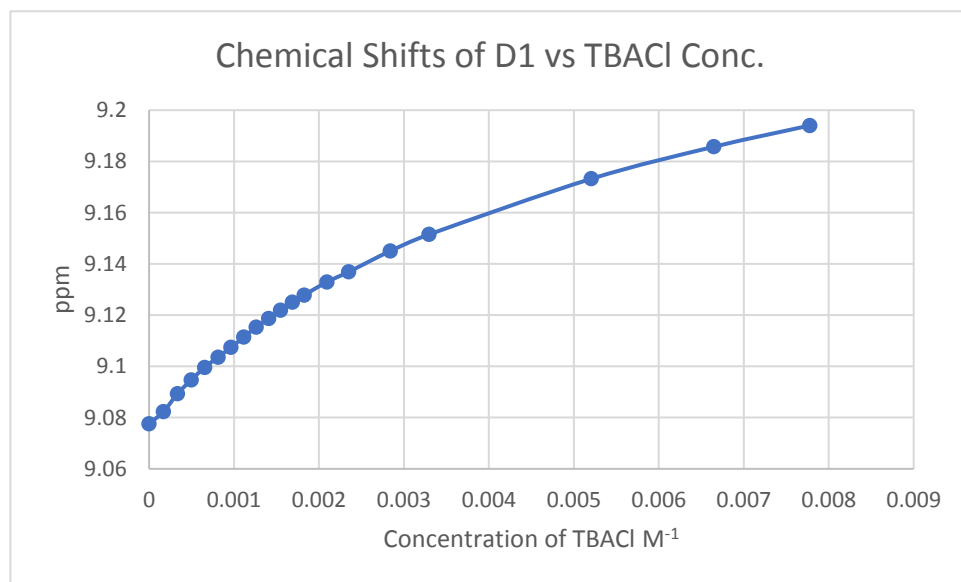
Calculated chemical shifts

Point	pH	D1	D2
1	-	8.52E+00	7.90E+00
2	-	8.53E+00	7.91E+00
3	-	8.54E+00	7.91E+00
4	-	8.56E+00	7.91E+00
5	-	8.57E+00	7.91E+00
6	-	8.58E+00	7.91E+00
7	-	8.59E+00	7.91E+00
8	-	8.60E+00	7.91E+00
9	-	8.61E+00	7.92E+00
10	-	8.61E+00	7.92E+00
11	-	8.63E+00	7.92E+00
12	-	8.64E+00	7.92E+00
13	-	8.65E+00	7.92E+00
14	-	8.66E+00	7.92E+00
15	-	8.67E+00	7.92E+00
16	-	8.68E+00	7.92E+00
17	-	8.68E+00	7.92E+00

18	-	8.69E+00	7.92E+00
19	-	8.70E+00	7.93E+00
20	-	8.72E+00	7.93E+00

Chemical shifts for each nucleus

species	D1	D2
H	8.52E+00	7.90E+00
GH	8.59E+00	7.92E+00
G ₂ H	8.85E+00	7.94E+00



G1HB and TBA⁺Cl⁻ (Experiment 3)

Species	Log beta	G	H	std. dev.
1	3.8238	1	1	0.2106
2	6.0416	2	1	0.2263

Converged in 1 iterations with sigma = 0.446288

Species concentrations/mol dm⁻³

Point	pH	T(TBACl)	T(G1HB)	F(TBACl)	F(G1HB)	species 1	species 2
1	-	0.00E+00	1.52E-03	5.64E-91	1.52E-03	5.72E-90	5.33E-178
2	-	2.66E-04	1.52E-03	2.76E-05	1.28E-03	2.36E-04	1.07E-06
3	-	5.26E-04	1.52E-03	6.39E-05	1.06E-03	4.53E-04	4.78E-06
4	-	7.82E-04	1.52E-03	1.12E-04	8.63E-04	6.45E-04	1.20E-05
5	-	1.03E-03	1.52E-03	1.76E-04	6.89E-04	8.09E-04	2.35E-05
6	-	1.28E-03	1.52E-03	2.59E-04	5.43E-04	9.38E-04	4.02E-05
7	-	1.52E-03	1.52E-03	3.63E-04	4.27E-04	1.03E-03	6.19E-05
8	-	1.76E-03	1.52E-03	4.85E-04	3.38E-04	1.09E-03	8.77E-05
9	-	1.99E-03	1.52E-03	6.23E-04	2.73E-04	1.13E-03	1.16E-04
10	-	2.22E-03	1.52E-03	7.72E-04	2.24E-04	1.15E-03	1.47E-04
11	-	2.66E-03	1.52E-03	1.09E-03	1.59E-04	1.15E-03	2.08E-04
12	-	3.09E-03	1.52E-03	1.42E-03	1.20E-04	1.13E-03	2.66E-04
13	-	3.50E-03	1.52E-03	1.75E-03	9.46E-05	1.11E-03	3.20E-04
14	-	3.90E-03	1.52E-03	2.09E-03	7.73E-05	1.07E-03	3.70E-04
15	-	4.28E-03	1.52E-03	2.41E-03	6.47E-05	1.04E-03	4.15E-04
16	-	4.66E-03	1.52E-03	2.74E-03	5.54E-05	1.01E-03	4.56E-04
17	-	5.02E-03	1.52E-03	3.05E-03	4.81E-05	9.79E-04	4.93E-04
18	-	5.37E-03	1.52E-03	3.36E-03	4.24E-05	9.51E-04	5.28E-04
19	-	6.35E-03	1.52E-03	4.25E-03	3.09E-05	8.76E-04	6.14E-04
20	-	7.53E-03	1.52E-03	5.33E-03	2.24E-05	7.97E-04	7.01E-04

Measured chemical shifts

Point	pH	D1	D2
1	-	8.52E+00	7.91E+00
2	-	8.53E+00	7.91E+00
3	-	8.54E+00	7.91E+00
4	-	8.56E+00	7.91E+00
5	-	8.57E+00	7.91E+00
6	-	8.58E+00	7.91E+00
7	-	8.59E+00	7.91E+00
8	-	8.60E+00	7.92E+00
9	-	8.61E+00	7.92E+00
10	-	8.62E+00	7.92E+00
11	-	8.63E+00	7.92E+00
12	-	8.64E+00	7.92E+00
13	-	8.65E+00	7.92E+00

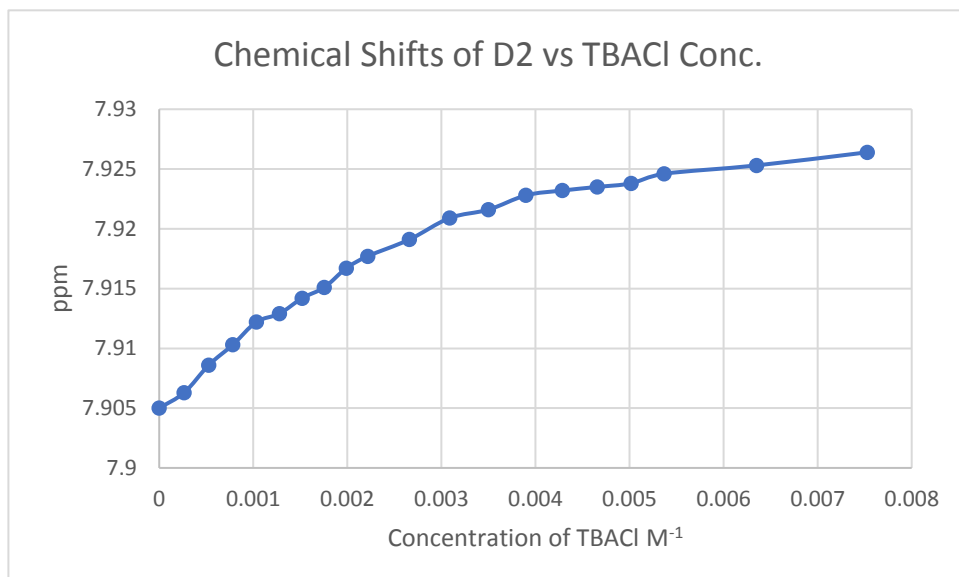
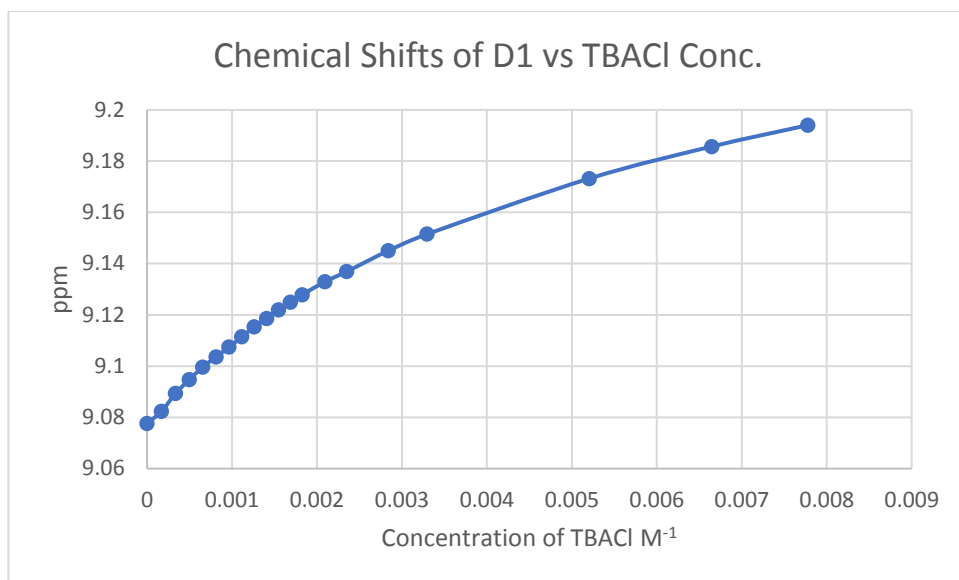
14	-	8.66E+00	7.92E+00
15	-	8.67E+00	7.92E+00
16	-	8.68E+00	7.92E+00
17	-	8.69E+00	7.92E+00
18	-	8.69E+00	7.92E+00
19	-	8.71E+00	7.93E+00
20	-	8.72E+00	7.93E+00

Calculated chemical shifts

Point	pH	D1	D2
1	-	8.52E+00	7.90E+00
2	-	8.53E+00	7.91E+00
3	-	8.54E+00	7.91E+00
4	-	8.56E+00	7.91E+00
5	-	8.57E+00	7.91E+00
6	-	8.58E+00	7.91E+00
7	-	8.59E+00	7.91E+00
8	-	8.60E+00	7.92E+00
9	-	8.61E+00	7.92E+00
10	-	8.62E+00	7.92E+00
11	-	8.63E+00	7.92E+00
12	-	8.64E+00	7.92E+00
13	-	8.65E+00	7.92E+00
14	-	8.66E+00	7.92E+00
15	-	8.67E+00	7.92E+00
16	-	8.68E+00	7.92E+00
17	-	8.69E+00	7.92E+00
18	-	8.69E+00	7.92E+00
19	-	8.71E+00	7.93E+00
20	-	8.72E+00	7.93E+00

Chemical shifts for each nucleus

species	D1	D2
H	8.52E+00	7.90E+00
GH	8.60E+00	7.92E+00
G ₂ H	8.86E+00	7.94E+00



G1HB and TBA⁺Br⁻ (Experiment 1)

Species	Log beta	G	H	std. dev.
1	3.0848	1	1	0.1308
2	4.9105	2	1	0.2195

Converged in 2 iterations with sigma = 0.020031

Species concentrations/mol dm⁻³

Point	pH	T(TBABr)	T(G1HB)	F(TBABr)	F(G1HB)	species 1	species 2
1	-	0.00E+00	1.56E-03	1.43E-90	1.56E-03	2.71E-90	2.59E-178
2	-	1.78E-04	1.56E-03	6.43E-05	1.45E-03	1.13E-04	4.87E-07
3	-	3.53E-04	1.56E-03	1.33E-04	1.34E-03	2.16E-04	1.93E-06

4	-	5.25E-04	1.56E-03	2.05E-04	1.24E-03	3.11E-04	4.27E-06
5	-	6.93E-04	1.56E-03	2.82E-04	1.16E-03	3.96E-04	7.47E-06
6	-	8.58E-04	1.56E-03	3.62E-04	1.07E-03	4.73E-04	1.15E-05
7	-	1.02E-03	1.56E-03	4.45E-04	1.00E-03	5.42E-04	1.62E-05
8	-	1.18E-03	1.56E-03	5.32E-04	9.34E-04	6.04E-04	2.15E-05
9	-	1.33E-03	1.56E-03	6.21E-04	8.73E-04	6.59E-04	2.74E-05
10	-	1.49E-03	1.56E-03	7.12E-04	8.18E-04	7.08E-04	3.37E-05
11	-	1.64E-03	1.56E-03	8.05E-04	7.68E-04	7.51E-04	4.05E-05
12	-	1.78E-03	1.56E-03	9.00E-04	7.22E-04	7.90E-04	4.76E-05
13	-	1.93E-03	1.56E-03	9.96E-04	6.80E-04	8.24E-04	5.49E-05
14	-	2.21E-03	1.56E-03	1.19E-03	6.08E-04	8.81E-04	7.02E-05
15	-	2.48E-03	1.56E-03	1.39E-03	5.48E-04	9.25E-04	8.59E-05
16	-	3.00E-03	1.56E-03	1.78E-03	4.56E-04	9.86E-04	1.18E-04
17	-	3.49E-03	1.56E-03	2.17E-03	3.88E-04	1.02E-03	1.48E-04
18	-	5.50E-03	1.56E-03	3.89E-03	2.24E-04	1.06E-03	2.76E-04
19	-	7.03E-03	1.56E-03	5.27E-03	1.61E-04	1.03E-03	3.64E-04
20	-	8.22E-03	1.56E-03	6.37E-03	1.30E-04	1.00E-03	4.27E-04

Measured chemical shifts

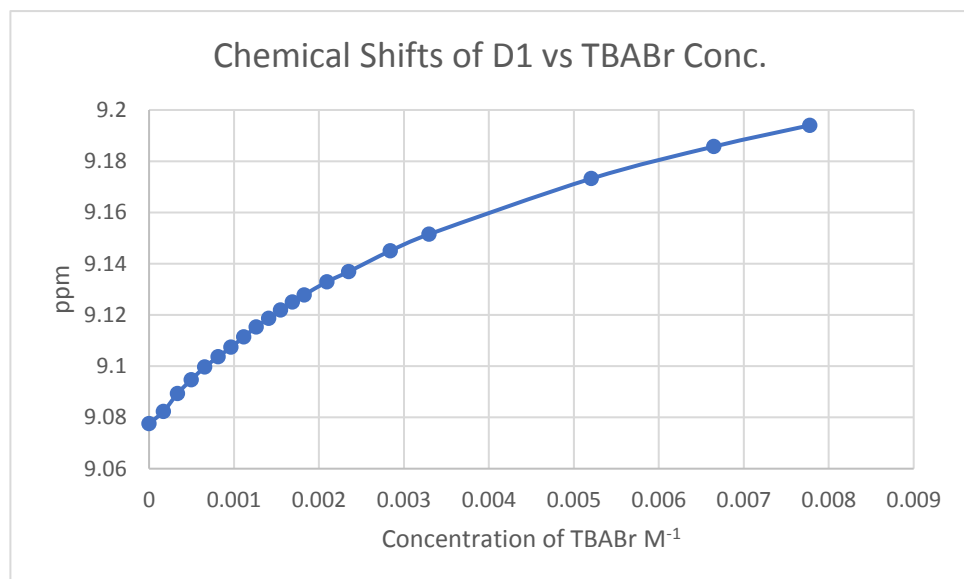
Point	pH	D1
1	-	9.08E+00
2	-	9.09E+00
3	-	9.10E+00
4	-	9.10E+00
5	-	9.11E+00
6	-	9.12E+00
7	-	9.12E+00
8	-	9.13E+00
9	-	9.13E+00
10	-	9.14E+00
11	-	9.15E+00
12	-	9.15E+00
13	-	9.15E+00
14	-	9.16E+00
15	-	9.17E+00
16	-	9.18E+00
17	-	9.19E+00
18	-	9.23E+00
19	-	9.24E+00
20	-	9.26E+00

Calculated chemical shifts

Point	pH	D1
1	-	9.08E+00
2	-	9.09E+00
3	-	9.10E+00
4	-	9.10E+00
5	-	9.11E+00
6	-	9.12E+00
7	-	9.12E+00
8	-	9.13E+00
9	-	9.13E+00
10	-	9.14E+00
11	-	9.15E+00
12	-	9.15E+00
13	-	9.15E+00
14	-	9.16E+00
15	-	9.17E+00
16	-	9.18E+00
17	-	9.19E+00
18	-	9.23E+00
19	-	9.24E+00
20	-	9.26E+00

Chemical shifts for each nucleus

species	D1
H	9.08E+00
GH	9.20E+00
G ₂ H	9.45E+00



G1HB and TBA⁺Br⁻ (Experiment 2)

Species	Log beta	G	H	std. dev.
1	2.9435	1	1	0.1809
2	4.674	2	1	0.3249

Converged in 3 iterations with sigma = 0.250421

Species concentrations/mol dm⁻³

Point	pH	T(TBABr)	T(G1HB)	F(TBABr)	F(G1HB)	species 1	species 2
1	-	0.00E+00	1.55E-03	1.59E-90	1.55E-03	2.17E-90	1.85E-178
2	-	2.76E-04	1.55E-03	1.23E-04	1.40E-03	1.51E-04	9.98E-07
3	-	5.46E-04	1.55E-03	2.56E-04	1.26E-03	2.83E-04	3.89E-06
4	-	8.12E-04	1.55E-03	3.97E-04	1.14E-03	3.98E-04	8.49E-06
5	-	1.07E-03	1.55E-03	5.46E-04	1.04E-03	4.97E-04	1.46E-05
6	-	1.33E-03	1.55E-03	7.01E-04	9.45E-04	5.82E-04	2.19E-05
7	-	1.58E-03	1.55E-03	8.62E-04	8.64E-04	6.54E-04	3.03E-05
8	-	1.82E-03	1.55E-03	1.03E-03	7.93E-04	7.16E-04	3.96E-05
9	-	2.06E-03	1.55E-03	1.20E-03	7.31E-04	7.68E-04	4.94E-05
10	-	2.30E-03	1.55E-03	1.37E-03	6.76E-04	8.13E-04	5.98E-05
11	-	2.76E-03	1.55E-03	1.72E-03	5.85E-04	8.82E-04	8.14E-05
12	-	3.21E-03	1.55E-03	2.07E-03	5.14E-04	9.32E-04	1.04E-04
13	-	3.63E-03	1.55E-03	2.42E-03	4.56E-04	9.67E-04	1.26E-04
14	-	4.05E-03	1.55E-03	2.76E-03	4.09E-04	9.92E-04	1.47E-04
15	-	4.45E-03	1.55E-03	3.10E-03	3.71E-04	1.01E-03	1.68E-04
16	-	4.84E-03	1.55E-03	3.44E-03	3.39E-04	1.02E-03	1.89E-04
17	-	5.21E-03	1.55E-03	3.76E-03	3.11E-04	1.03E-03	2.08E-04
18	-	5.57E-03	1.55E-03	4.09E-03	2.88E-04	1.03E-03	2.27E-04
19	-	6.59E-03	1.55E-03	5.00E-03	2.36E-04	1.04E-03	2.78E-04
20	-	7.82E-03	1.55E-03	6.12E-03	1.90E-04	1.02E-03	3.37E-04

Measured chemical shifts

Point	pH	D1
1	-	9.07E+00
2	-	9.08E+00
3	-	9.09E+00
4	-	9.10E+00
5	-	9.12E+00
6	-	9.13E+00
7	-	9.14E+00
8	-	9.14E+00
9	-	9.14E+00
10	-	9.15E+00
11	-	9.16E+00
12	-	9.17E+00

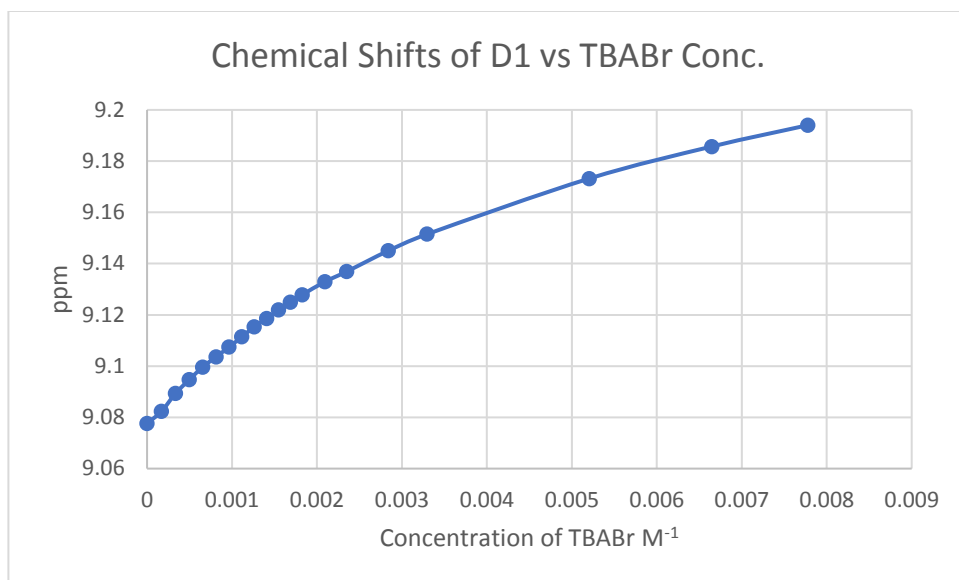
13	-	9.19E+00
14	-	9.19E+00
15	-	9.20E+00
16	-	9.21E+00
17	-	9.22E+00
18	-	9.22E+00
19	-	9.23E+00
20	-	9.25E+00

Calculated chemical shifts

Point	pH	D1
1	-	9.07E+00
2	-	9.08E+00
3	-	9.10E+00
4	-	9.11E+00
5	-	9.12E+00
6	-	9.12E+00
7	-	9.13E+00
8	-	9.14E+00
9	-	9.15E+00
10	-	9.15E+00
11	-	9.17E+00
12	-	9.18E+00
13	-	9.19E+00
14	-	9.19E+00
15	-	9.20E+00
16	-	9.21E+00
17	-	9.21E+00
18	-	9.22E+00
19	-	9.23E+00
20	-	9.25E+00

Chemical shifts for each nucleus

species	D1
H	9.07E+00
GH	9.20E+00
G ₂ H	9.51E+00



G1HB and TBA⁺Br⁻ (Experiment 3)

Species	Log beta	G	H	std. dev.
1	3.1476	1	1	0.1173
2	4.9113	2	1	0.1883

Converged in 3 iterations with sigma = 0.1820

Species concentrations/mol dm⁻³

Point	pH	T(TBABr)	T(G1HB)	F(TBABr)	F(G1HB)	species 1	species 2
1	-	0.00E+00	1.55E-03	1.34E-90	1.55E-03	2.93E-90	2.28E-178
2	-	2.76E-04	1.55E-03	9.38E-05	1.37E-03	1.80E-04	9.81E-07
3	-	5.46E-04	1.55E-03	2.00E-04	1.21E-03	3.39E-04	3.93E-06
4	-	8.12E-04	1.55E-03	3.18E-04	1.06E-03	4.76E-04	8.79E-06
5	-	1.07E-03	1.55E-03	4.48E-04	9.41E-04	5.93E-04	1.54E-05
6	-	1.33E-03	1.55E-03	5.89E-04	8.35E-04	6.91E-04	2.36E-05
7	-	1.58E-03	1.55E-03	7.39E-04	7.44E-04	7.72E-04	3.31E-05
8	-	1.82E-03	1.55E-03	8.97E-04	6.66E-04	8.39E-04	4.37E-05
9	-	2.06E-03	1.55E-03	1.06E-03	6.00E-04	8.94E-04	5.50E-05
10	-	2.30E-03	1.55E-03	1.23E-03	5.44E-04	9.38E-04	6.69E-05
11	-	2.76E-03	1.55E-03	1.57E-03	4.54E-04	1.00E-03	9.17E-05
12	-	3.21E-03	1.55E-03	1.93E-03	3.86E-04	1.05E-03	1.17E-04
13	-	3.63E-03	1.55E-03	2.28E-03	3.35E-04	1.07E-03	1.42E-04
14	-	4.05E-03	1.55E-03	2.63E-03	2.95E-04	1.09E-03	1.66E-04
15	-	4.45E-03	1.55E-03	2.97E-03	2.63E-04	1.10E-03	1.89E-04
16	-	4.84E-03	1.55E-03	3.31E-03	2.37E-04	1.10E-03	2.12E-04
17	-	5.21E-03	1.55E-03	3.64E-03	2.15E-04	1.10E-03	2.33E-04
18	-	5.57E-03	1.55E-03	3.97E-03	1.97E-04	1.10E-03	2.53E-04
19	-	6.59E-03	1.55E-03	4.89E-03	1.58E-04	1.08E-03	3.08E-04
20	-	7.82E-03	1.55E-03	6.03E-03	1.25E-04	1.06E-03	3.69E-04

Measured chemical shifts

Point	pH	D1
1	-	9.07E+00
2	-	9.08E+00
3	-	9.10E+00
4	-	9.11E+00
5	-	9.12E+00
6	-	9.13E+00
7	-	9.14E+00
8	-	9.14E+00
9	-	9.15E+00
10	-	9.15E+00
11	-	9.17E+00
12	-	9.18E+00
13	-	9.19E+00
14	-	9.19E+00
15	-	9.20E+00
16	-	9.21E+00
17	-	9.22E+00
18	-	9.22E+00
19	-	9.24E+00
20	-	9.25E+00

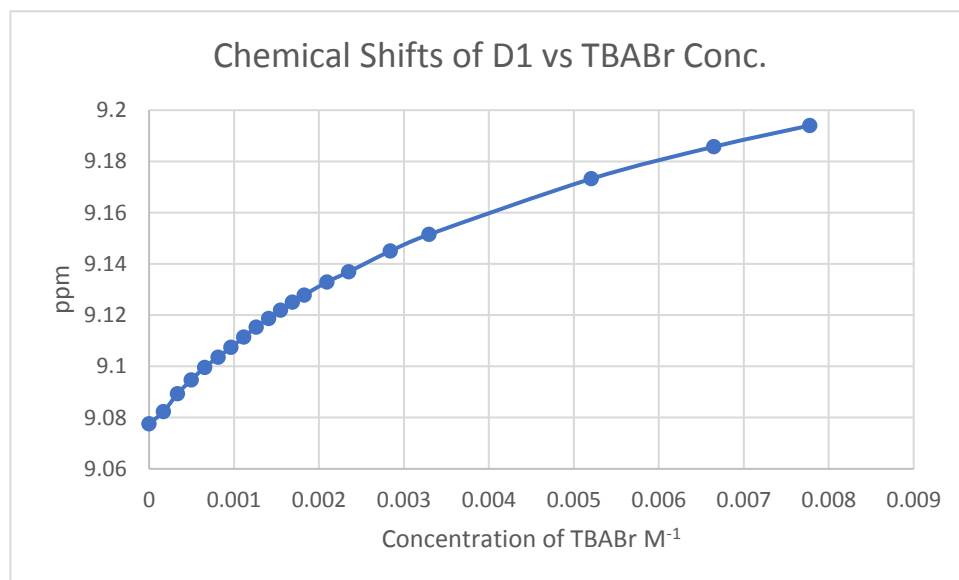
Calculated chemical shifts

Point	pH	D1
1	-	9.08E+00
2	-	9.09E+00
3	-	9.10E+00
4	-	9.11E+00
5	-	9.12E+00
6	-	9.13E+00
7	-	9.14E+00
8	-	9.14E+00
9	-	9.15E+00
10	-	9.16E+00
11	-	9.17E+00
12	-	9.18E+00
13	-	9.19E+00
14	-	9.19E+00
15	-	9.20E+00
16	-	9.21E+00
17	-	9.21E+00

18	-	9.22E+00
19	-	9.23E+00
20	-	9.25E+00

Chemical shifts for each nucleus

species	D1
H	9.08E+00
GH	9.18E+00
G ₂ H	9.52E+00



G1HB and TBAI⁻ (Experiment 1)

Species	Log beta	G	H	std. dev.
1	3.0582	1	1	0.0596
2	4.4667	2	1	0.1941

Converged in 2 iterations with sigma = 0.044285

Species concentrations/mol dm⁻³

Point	pH	T(TBAI)	T(G1HB)	F(TBAI)	F(G1HB)	species 1	species 2
1	-	0.00E+00	1.60E-03	1.48E-90	1.60E-03	2.70E-90	1.02E-178
2	-	1.69E-04	1.60E-03	6.22E-05	1.49E-03	1.06E-04	1.69E-07
3	-	3.34E-04	1.60E-03	1.28E-04	1.39E-03	2.04E-04	6.71E-07
4	-	4.96E-04	1.60E-03	1.98E-04	1.30E-03	2.95E-04	1.50E-06
5	-	6.55E-04	1.60E-03	2.72E-04	1.22E-03	3.78E-04	2.63E-06
6	-	8.11E-04	1.60E-03	3.48E-04	1.14E-03	4.54E-04	4.06E-06
7	-	9.64E-04	1.60E-03	4.28E-04	1.07E-03	5.24E-04	5.75E-06
8	-	1.11E-03	1.60E-03	5.11E-04	1.00E-03	5.87E-04	7.69E-06
9	-	1.26E-03	1.60E-03	5.97E-04	9.45E-04	6.45E-04	9.86E-06
10	-	1.41E-03	1.60E-03	6.85E-04	8.90E-04	6.97E-04	1.22E-05

11	-	1.55E-03	1.60E-03	7.75E-04	8.40E-04	7.44E-04	1.48E-05
12	-	1.69E-03	1.60E-03	8.66E-04	7.95E-04	7.87E-04	1.75E-05
13	-	1.82E-03	1.60E-03	9.58E-04	7.53E-04	8.26E-04	2.03E-05
14	-	2.09E-03	1.60E-03	1.15E-03	6.81E-04	8.92E-04	2.62E-05
15	-	2.35E-03	1.60E-03	1.34E-03	6.20E-04	9.47E-04	3.24E-05
16	-	2.84E-03	1.60E-03	1.72E-03	5.24E-04	1.03E-03	4.53E-05
17	-	3.30E-03	1.60E-03	2.09E-03	4.54E-04	1.09E-03	5.83E-05
18	-	5.20E-03	1.60E-03	3.77E-03	2.79E-04	1.20E-03	1.16E-04
19	-	6.65E-03	1.60E-03	5.10E-03	2.11E-04	1.23E-03	1.60E-04
20	-	7.77E-03	1.60E-03	6.16E-03	1.75E-04	1.23E-03	1.94E-04

Measured chemical shifts

Point	pH	D1
1	-	9.08E+00
2	-	9.08E+00
3	-	9.09E+00
4	-	9.09E+00
5	-	9.10E+00
6	-	9.10E+00
7	-	9.11E+00
8	-	9.11E+00
9	-	9.12E+00
10	-	9.12E+00
11	-	9.12E+00
12	-	9.13E+00
13	-	9.13E+00
14	-	9.13E+00
15	-	9.14E+00
16	-	9.15E+00
17	-	9.15E+00
18	-	9.17E+00
19	-	9.19E+00
20	-	9.19E+00

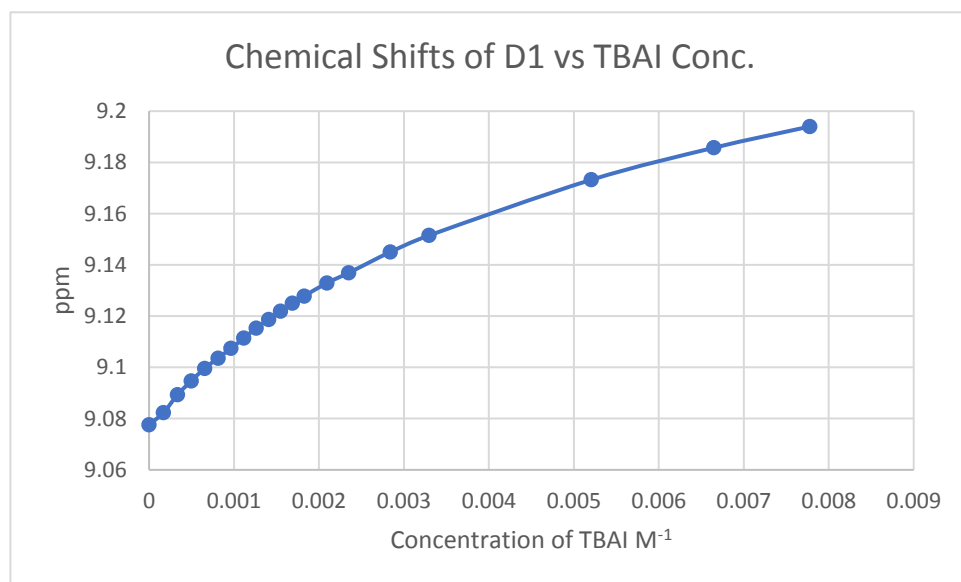
Calculated chemical shifts

Point	pH	D1
1	-	9.08E+00
2	-	9.08E+00
3	-	9.09E+00
4	-	9.09E+00
5	-	9.10E+00
6	-	9.10E+00
7	-	9.11E+00

8	-	9.11E+00
9	-	9.12E+00
10	-	9.12E+00
11	-	9.12E+00
12	-	9.12E+00
13	-	9.13E+00
14	-	9.13E+00
15	-	9.14E+00
16	-	9.15E+00
17	-	9.15E+00
18	-	9.17E+00
19	-	9.19E+00
20	-	9.19E+00

Chemical shifts for each nucleus

species	D1
H	9.08E+00
GH	9.16E+00
G ₂ H	9.49E+00



G1HB and TBA⁺I⁻ (Experiment 2)

Species	Log beta	G	H	std. dev.
1	2.9802	1	1	0.0369
2	4.4742	2	1	0.1188

Converged in 3 iterations with sigma = 0.038141

Species concentrations/mol dm⁻³

Point	pH	T(TBAI)	T(G1HB)	F(TBAI)	F(G1HB)	species 1	species 2
1	-	0.00E+00	1.52E-03	1.54E-90	1.52E-03	2.23E-90	1.07E-178
2	-	2.73E-04	1.52E-03	1.18E-04	1.37E-03	1.54E-04	5.65E-07
3	-	5.40E-04	1.52E-03	2.46E-04	1.23E-03	2.89E-04	2.22E-06
4	-	8.02E-04	1.52E-03	3.85E-04	1.11E-03	4.07E-04	4.89E-06
5	-	1.06E-03	1.52E-03	5.32E-04	1.00E-03	5.10E-04	8.46E-06
6	-	1.31E-03	1.52E-03	6.88E-04	9.10E-04	5.98E-04	1.28E-05
7	-	1.56E-03	1.52E-03	8.49E-04	8.30E-04	6.73E-04	1.78E-05
8	-	1.80E-03	1.52E-03	1.02E-03	7.60E-04	7.38E-04	2.34E-05
9	-	2.04E-03	1.52E-03	1.19E-03	6.99E-04	7.93E-04	2.94E-05
10	-	2.27E-03	1.52E-03	1.36E-03	6.45E-04	8.40E-04	3.57E-05
11	-	2.73E-03	1.52E-03	1.72E-03	5.58E-04	9.14E-04	4.89E-05
12	-	3.17E-03	1.52E-03	2.07E-03	4.89E-04	9.69E-04	6.27E-05
13	-	3.59E-03	1.52E-03	2.43E-03	4.35E-04	1.01E-03	7.65E-05
14	-	4.00E-03	1.52E-03	2.78E-03	3.91E-04	1.04E-03	9.02E-05
15	-	4.40E-03	1.52E-03	3.13E-03	3.55E-04	1.06E-03	1.04E-04
16	-	4.78E-03	1.52E-03	3.47E-03	3.26E-04	1.08E-03	1.17E-04
17	-	5.15E-03	1.52E-03	3.80E-03	3.01E-04	1.09E-03	1.29E-04
18	-	5.51E-03	1.52E-03	4.12E-03	2.79E-04	1.10E-03	1.41E-04
19	-	6.52E-03	1.52E-03	5.05E-03	2.31E-04	1.11E-03	1.76E-04
20	-	7.72E-03	1.52E-03	6.18E-03	1.89E-04	1.12E-03	2.15E-04

Measured chemical shifts

Point	pH	D1	D2
1	-	9.08E+00	8.46E+00
2	-	9.09E+00	8.47E+00
3	-	9.10E+00	8.47E+00
4	-	9.10E+00	8.47E+00
5	-	9.11E+00	8.47E+00
6	-	9.12E+00	8.48E+00
7	-	9.12E+00	8.48E+00
8	-	9.13E+00	8.48E+00
9	-	9.13E+00	8.48E+00
10	-	9.14E+00	8.48E+00
11	-	9.14E+00	8.48E+00
12	-	9.15E+00	8.49E+00
13	-	9.16E+00	8.49E+00
14	-	9.16E+00	8.49E+00
15	-	9.17E+00	8.49E+00
16	-	9.17E+00	8.49E+00
17	-	9.17E+00	8.49E+00
18	-	9.18E+00	8.49E+00

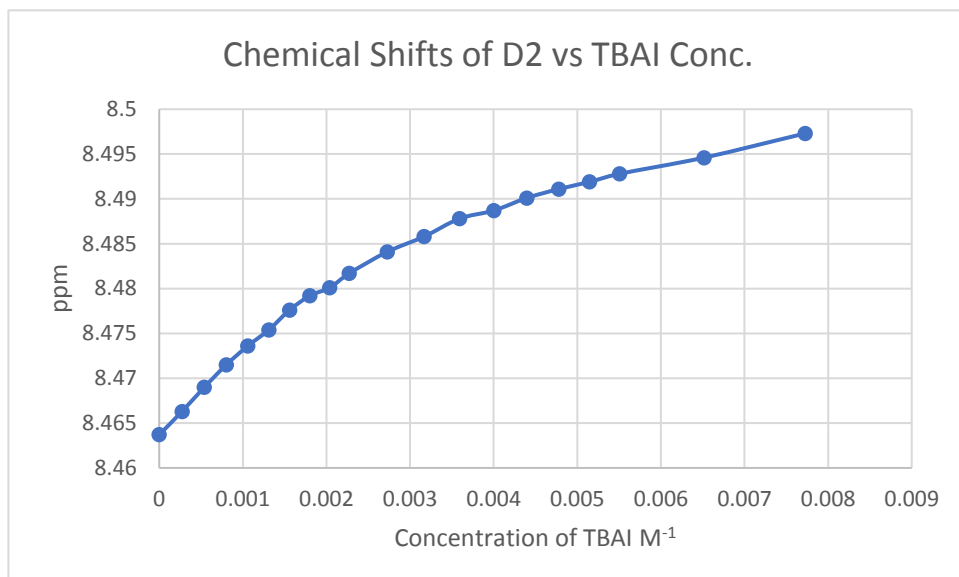
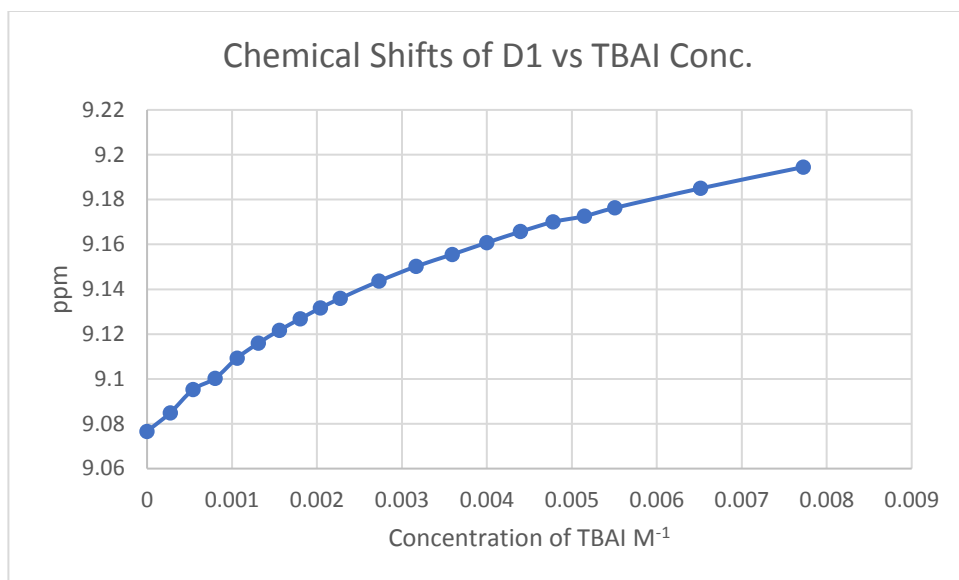
19	-	9.19E+00	8.49E+00
20	-	9.19E+00	8.50E+00

Calculated chemical shifts

Point	pH	D1	D2
1	-	9.08E+00	8.46E+00
2	-	9.09E+00	8.47E+00
3	-	9.10E+00	8.47E+00
4	-	9.10E+00	8.47E+00
5	-	9.11E+00	8.47E+00
6	-	9.12E+00	8.48E+00
7	-	9.12E+00	8.48E+00
8	-	9.13E+00	8.48E+00
9	-	9.13E+00	8.48E+00
10	-	9.14E+00	8.48E+00
11	-	9.14E+00	8.48E+00
12	-	9.15E+00	8.49E+00
13	-	9.16E+00	8.49E+00
14	-	9.16E+00	8.49E+00
15	-	9.17E+00	8.49E+00
16	-	9.17E+00	8.49E+00
17	-	9.17E+00	8.49E+00
18	-	9.18E+00	8.49E+00
19	-	9.19E+00	8.50E+00
20	-	9.19E+00	8.50E+00

Chemical shifts for each nucleus

species	D1	D2	S1
H	9.08E+00	8.46E+00	8.34E+00
GH	9.17E+00	8.49E+00	0.00E+00
G ₂ H	9.43E+00	8.55E+00	0.00E+00



G1HB and TBAI⁺ (Experiment 3)

Species	Log beta	G	H	std. dev.
1	3.0001	1	1	0.0603
2	4.6269	2	1	0.154

Converged in 1 iterations with sigma = 0.061647

Species concentrations/mol dm^{-3}

Point	pH	T(TBAI)	T(G1HB)	F(TBAI)	F(G1HB)	species 1	species 2
1	-	0.00E+00	1.52E-03	7.38E-91	1.52E-03	4.89E-90	3.89E-178
2	-	2.73E-04	1.52E-03	4.09E-05	1.29E-03	2.30E-04	1.01E-06
3	-	5.40E-04	1.52E-03	9.32E-05	1.08E-03	4.38E-04	4.40E-06
4	-	8.02E-04	1.52E-03	1.60E-04	8.90E-04	6.20E-04	1.07E-05

5	-	1.06E-03	1.52E-03	2.45E-04	7.27E-04	7.74E-04	2.04E-05
6	-	1.31E-03	1.52E-03	3.48E-04	5.91E-04	8.96E-04	3.36E-05
7	-	1.56E-03	1.52E-03	4.70E-04	4.83E-04	9.88E-04	5.01E-05
8	-	1.80E-03	1.52E-03	6.09E-04	3.98E-04	1.05E-03	6.92E-05
9	-	2.04E-03	1.52E-03	7.60E-04	3.32E-04	1.10E-03	9.01E-05
10	-	2.27E-03	1.52E-03	9.22E-04	2.81E-04	1.13E-03	1.12E-04
11	-	2.73E-03	1.52E-03	1.26E-03	2.10E-04	1.15E-03	1.57E-04
12	-	3.17E-03	1.52E-03	1.61E-03	1.65E-04	1.16E-03	2.01E-04
13	-	3.59E-03	1.52E-03	1.96E-03	1.34E-04	1.14E-03	2.42E-04
14	-	4.00E-03	1.52E-03	2.31E-03	1.12E-04	1.13E-03	2.81E-04
15	-	4.40E-03	1.52E-03	2.65E-03	9.59E-05	1.11E-03	3.17E-04
16	-	4.78E-03	1.52E-03	2.99E-03	8.35E-05	1.09E-03	3.50E-04
17	-	5.15E-03	1.52E-03	3.32E-03	7.37E-05	1.07E-03	3.81E-04
18	-	5.51E-03	1.52E-03	3.64E-03	6.59E-05	1.04E-03	4.10E-04
19	-	6.52E-03	1.52E-03	4.56E-03	4.97E-05	9.86E-04	4.85E-04
20	-	7.72E-03	1.52E-03	5.68E-03	3.72E-05	9.20E-04	5.63E-04

Measured chemical shifts

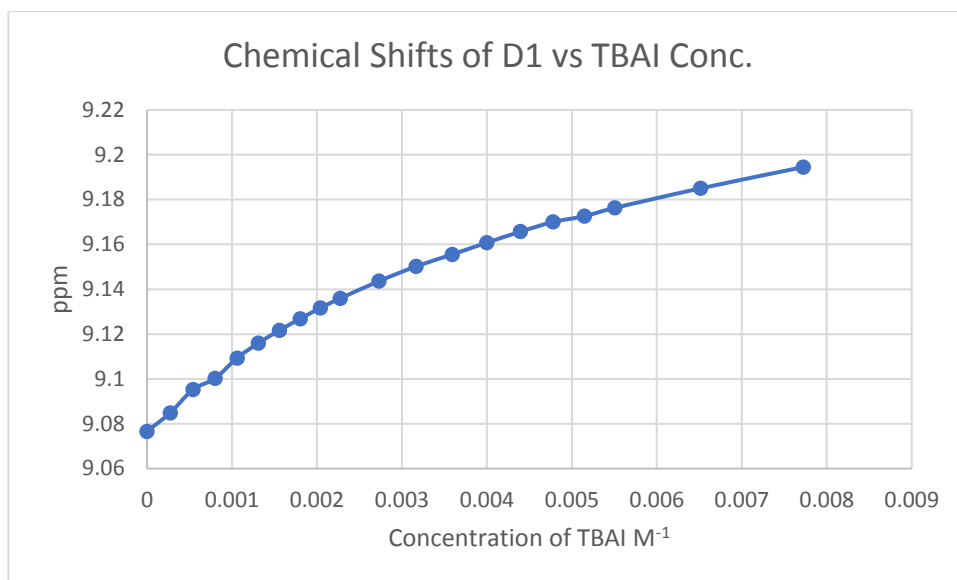
Point	pH	D1
1	-	9.08E+00
2	-	9.08E+00
3	-	9.10E+00
4	-	9.10E+00
5	-	9.11E+00
6	-	9.12E+00
7	-	9.12E+00
8	-	9.13E+00
9	-	9.13E+00
10	-	9.14E+00
11	-	9.14E+00
12	-	9.15E+00
13	-	9.16E+00
14	-	9.16E+00
15	-	9.17E+00
16	-	9.17E+00
17	-	9.17E+00
18	-	9.18E+00
19	-	9.19E+00
20	-	9.19E+00

Calculated chemical shifts

Point	pH	D1
1	-	9.08E+00
2	-	9.09E+00
3	-	9.09E+00
4	-	9.10E+00
5	-	9.11E+00
6	-	9.12E+00
7	-	9.12E+00
8	-	9.13E+00
9	-	9.13E+00
10	-	9.14E+00
11	-	9.14E+00
12	-	9.15E+00
13	-	9.16E+00
14	-	9.16E+00
15	-	9.17E+00
16	-	9.17E+00
17	-	9.17E+00
18	-	9.18E+00
19	-	9.19E+00
20	-	9.19E+00

Chemical shifts for each nucleus

species	D1
H	9.08E+00
GH	9.13E+00
G ₂ H	9.30E+00



Procedure for Proton-Deuterium Exchange

Initial spectra were acquired with 500 μL of **G2XB** and **G2HB** with a concentration of 4 mM in CDCl_3 at -8°C . To this was added 2 μL of D_2O marking time = 0. Spectra were acquired every 30 seconds until the disappearance of the proton signal into the baseline. To minimize variability, a constant baseline correction was applied.

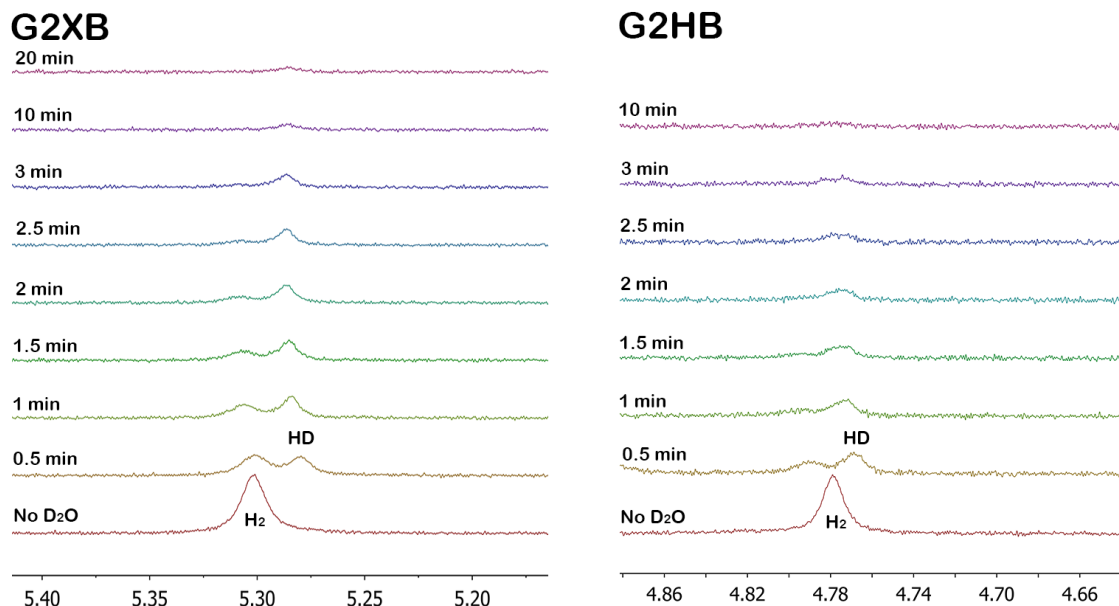


Figure S23. Stacked ^1H NMR spectra of H/D exchange with **G2XB** and **G2HB**. The H_2 signal of **G2XB** disappeared after 3 minutes, whereas the H_2 signal of **G2HB** is observed for only 1.5 minutes. The HD signal of **G2HB** disappeared after 10 minutes after addition of D_2O , while the same signal for **G2XB** persists even after 20 minutes.

Variable Temperature ^1H NMR

Variable temperature ^1H NMR spectra of **G2XB** (2.08 mM in CDCl_3) and **G2HB** (2.11 mM in CDCl_3) were taken at 10°C increments. Spectra were collected from -10°C up to 60°C shown in below.

Amine proton signals display a shift in resonance upon changes in temperature. Both **G2XB** ($-1.329 \times 10^{-3} \text{ ppm K}^{-1}$) and **G2HB** ($-1.247 \times 10^{-3} \text{ ppm K}^{-1}$) amine signals displayed small upfield shifts reminiscent of intramolecular H-bing. **G2XB** exhibits a slightly greater

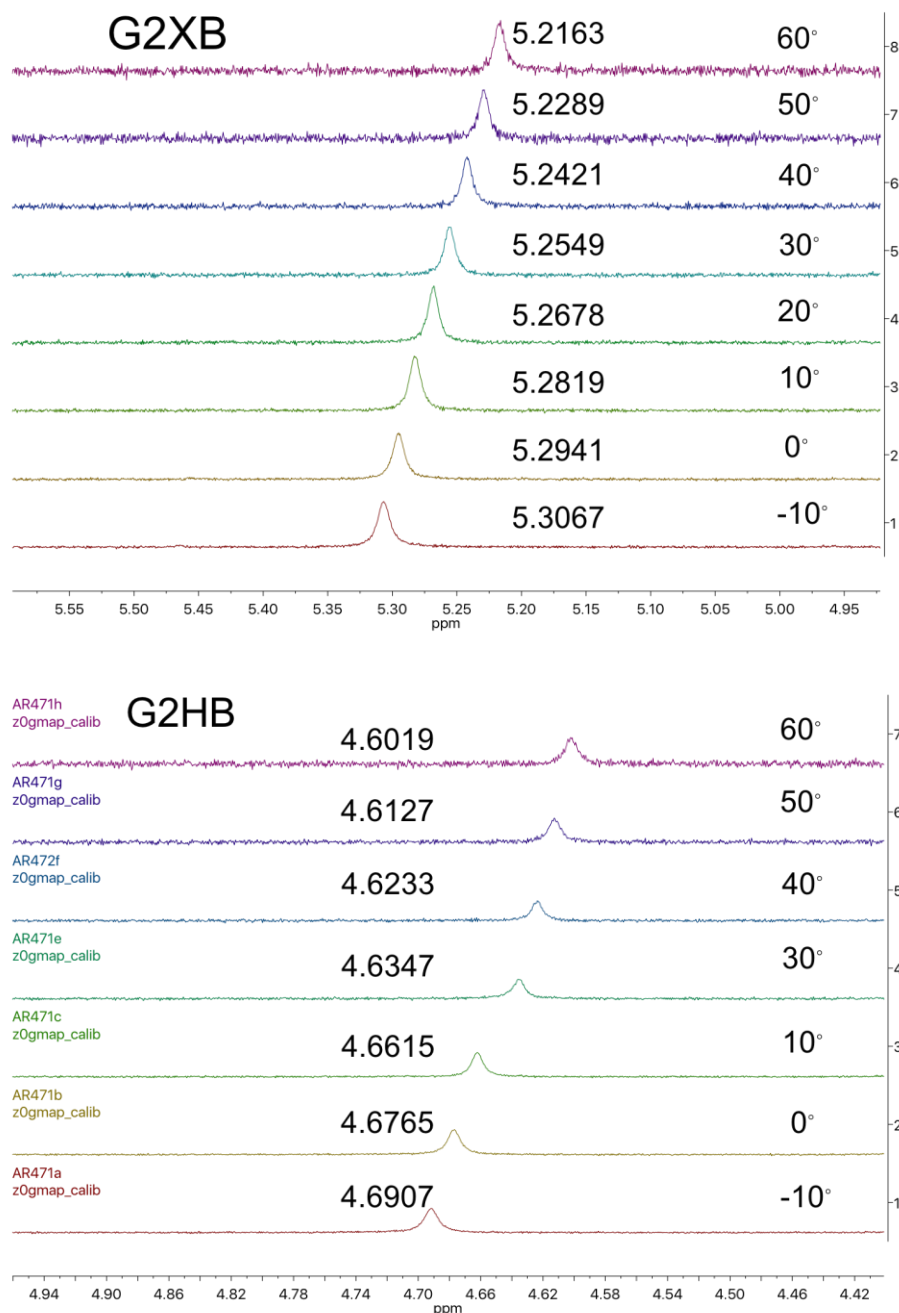


Figure S24. Stacked ^1H NMR spectra of the NH_2 resonances of **G2XB** and **G2HB**.

upfield shift in NH₂ proton resonance which correlate to intramolecular HB to XB preorganization.

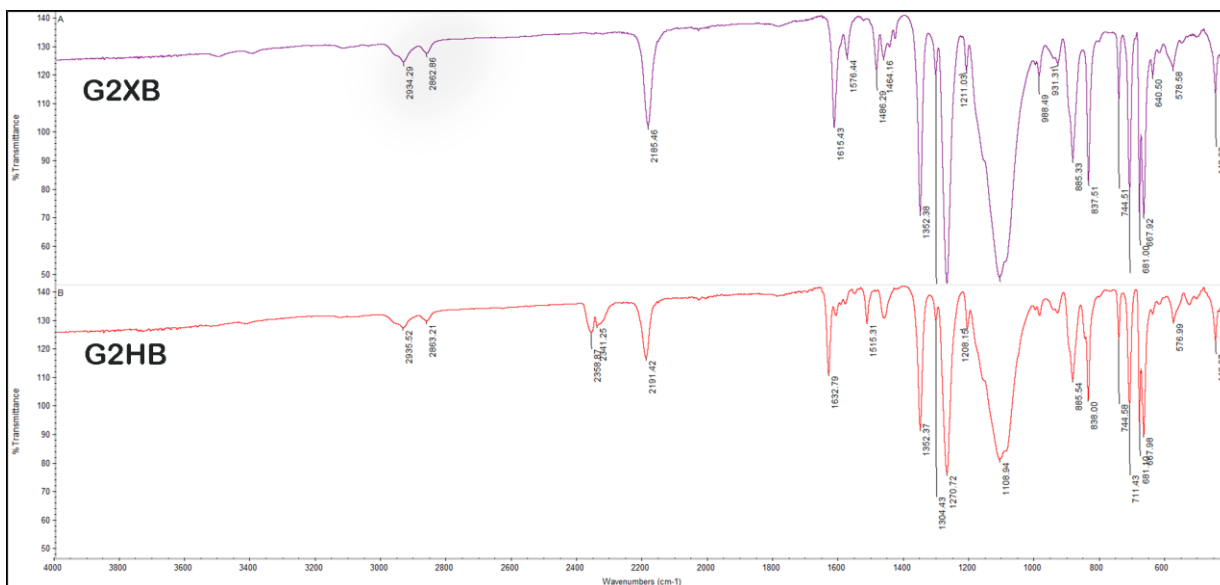
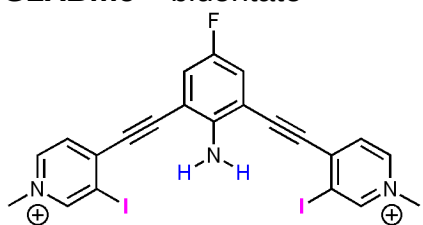


Figure S25. IR data of G2XB and G2HB.

General Computational Information

Calculations were carried out with the Gaussian '09 suite of programs using B3LYP functional employing the 6-31+G(d,p) basis set for all atoms except nitrogen and iodine. For which nitrogen—aug-cc-pVTZ basis set and iodide— LANL2DZdp and effective core potential (ECP) were used. The LANL2DZdp ECP basis set was downloaded from the EMSL Basis Set Exchange (<https://bse.pnl.gov/bse/portal>). Crystal structures of G2XBme and G1XBme were employed as a starting point for optimization.

G2XBme²⁺-bidentate

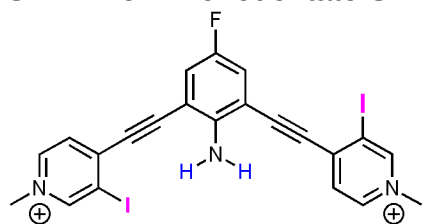


Coordinates for G2XBme²⁺-bidentate:

2	1			
I	3.58390000	-2.10992000	-0.00315000	
F	0.00003000	5.95285000	-0.00265000	
N	0.00000000	0.43340000	0.00022000	
H	0.86420000	-0.08224000	-0.00004000	
H	-0.86421000	-0.08223000	-0.00005000	
N	7.46036000	-0.26288000	-0.00263000	
C	4.84095000	0.72302000	0.00066000	
C	5.10564000	-0.67599000	-0.00027000	

C	3.54736000	1.27087000	0.00002000
C	1.22880000	2.52038000	-0.00093000
C	2.46828000	1.84753000	-0.00047000
C	6.41736000	-1.12233000	-0.00105000
H	6.66683000	-2.17589000	-0.00153000
C	0.00001000	1.78238000	-0.00059000
C	-2.46827000	1.84756000	-0.00050000
C	1.20939000	3.93058000	-0.00160000
H	2.13813000	4.48998000	-0.00185000
C	-1.22879000	2.52040000	-0.00094000
C	-3.54736000	1.27093000	-0.00006000
C	0.00002000	4.60678000	-0.00197000
C	5.96936000	1.58514000	-0.00005000
H	5.82786000	2.65927000	-0.00135000
C	7.24596000	1.07644000	-0.00118000
H	8.12686000	1.70708000	-0.00217000
C	-1.20935000	3.93059000	-0.00162000
H	-2.13808000	4.49001000	-0.00189000
N	-7.46039000	-0.26278000	-0.00294000
C	-4.84096000	0.72310000	0.00055000
C	-7.24598000	1.07652000	-0.00145000
H	-8.12684000	1.70721000	-0.00252000
C	-5.96935000	1.58521000	-0.00024000
C	8.85204000	-0.77428000	0.02542000
H	9.27652000	-0.61192000	1.01894000
H	9.44102000	-0.24414000	-0.72438000
H	8.84678000	-1.83882000	-0.20391000
C	-5.10567000	-0.67593000	-0.00038000
C	-6.41737000	-1.12224000	-0.00123000
H	-6.66688000	-2.17580000	-0.00171000
C	-8.85188000	-0.77463000	0.02630000
H	-9.27169000	-0.62311000	1.02355000
H	-8.84765000	-1.83659000	-0.21479000
H	-9.44443000	-0.23644000	-0.71483000
I	-3.58393000	-2.10985000	-0.00325000
H	-5.82786000	2.65934000	-0.00162000

G2XBme²⁺-monodentate S

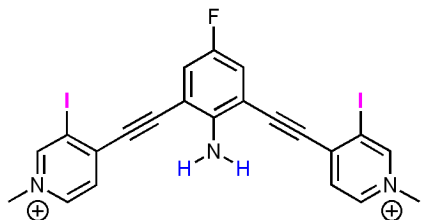


Coordinates for G2XBme²⁺-monodentate S:

2	1			
I	-4.62041000	-2.19672000	0.00290000	
F	0.67344000	4.85291000	-0.00491000	
N	-0.59257000	-0.51993000	-0.00079000	
H	-1.55206000	-0.82333000	-0.00040000	
H	0.12840000	-1.21958000	-0.00031000	

N	-7.99989000	0.45248000	0.00636000
C	-5.22850000	0.84264000	-0.00029000
C	-5.79224000	-0.46488000	0.00145000
C	-3.84638000	1.09386000	-0.00119000
C	-1.30683000	1.79221000	-0.00234000
C	-2.66639000	1.41726000	-0.00176000
C	-7.16979000	-0.61401000	0.00393000
H	-7.64330000	-1.58766000	0.00511000
C	-0.27924000	0.79343000	-0.00171000
C	2.14995000	0.30199000	-0.00120000
C	-0.96715000	3.16128000	-0.00342000
H	-1.74404000	3.91751000	-0.00391000
C	1.08485000	1.22977000	-0.00204000
C	3.12222000	-0.44039000	-0.00056000
C	0.36445000	3.54247000	-0.00386000
C	-6.14136000	1.93040000	0.00122000
H	-5.76867000	2.94769000	0.00179000
C	-7.49820000	1.71268000	0.00407000
H	-8.22021000	2.52040000	0.00579000
C	1.38706000	2.60720000	-0.00316000
H	2.41968000	2.93717000	-0.00344000
N	6.51966000	-2.91710000	0.00959000
C	4.26924000	-1.25392000	0.00042000
C	6.67449000	-1.57363000	0.00570000
H	7.69502000	-1.21154000	0.00710000
C	5.58942000	-0.71174000	0.00216000
C	-9.46980000	0.25789000	-0.01783000
H	-9.85301000	0.52398000	-1.00570000
H	-9.92540000	0.89250000	0.74374000
H	-9.69623000	-0.78545000	0.19656000
C	4.15929000	-2.66736000	0.00328000
C	5.28043000	-3.46437000	0.00687000
H	5.22905000	-4.54623000	0.00955000
C	7.71188000	-3.79790000	-0.03014000
H	7.91733000	-4.08406000	-1.06465000
H	7.51727000	-4.68609000	0.57130000
H	8.56573000	-3.26196000	0.38283000
H	3.18267000	-3.13580000	0.00515000
I	5.97196000	1.34103000	0.00333000

G2XBme²⁺-monodentate W

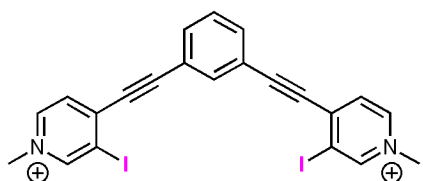


Coordinates for G2XBme²⁺-monodentate W:

2	1		
I	-5.97239000	-1.57261000	-0.00665000
F	0.00000000	-3.80287000	0.00000000
N	-7.45282000	2.45734000	-0.00628000

N	0.00000000	1.71786000	-0.00002000
H	0.86229000	2.23316000	0.00003000
C	-7.30530000	1.11308000	-0.00454000
H	-8.21984000	0.53327000	-0.00658000
C	-6.05579000	0.51380000	-0.00228000
C	-4.88916000	1.33573000	0.00038000
C	-5.09600000	2.73832000	-0.00025000
H	-4.24795000	3.41215000	-0.00123000
C	-6.36616000	3.26630000	-0.00265000
H	-6.55646000	4.33255000	-0.00359000
C	-3.58979000	0.79790000	0.00026000
C	-2.47595000	0.29216000	0.00002000
C	-1.22808000	-0.36977000	-0.00004000
C	-1.20910000	-1.78009000	-0.00005000
H	-2.13944000	-2.33649000	-0.00008000
C	0.00000000	-2.45619000	0.00000000
C	0.00000000	0.36629000	-0.00001000
C	-8.81064000	3.05189000	0.03409000
H	-9.06941000	3.29561000	1.06749000
H	-9.52622000	2.33569000	-0.36808000
H	-8.82103000	3.95507000	-0.57645000
I	5.97238000	-1.57261000	0.00666000
N	7.45283000	2.45734000	0.00630000
H	-0.86230000	2.23316000	-0.00010000
C	7.30530000	1.11308000	0.00456000
H	8.21984000	0.53326000	0.00661000
C	6.05579000	0.51380000	0.00229000
C	4.88916000	1.33574000	-0.00040000
C	5.09600000	2.73832000	0.00024000
H	4.24795000	3.41215000	0.00121000
C	6.36616000	3.26630000	0.00265000
H	6.55646000	4.33255000	0.00359000
C	3.58979000	0.79790000	-0.00028000
C	2.47595000	0.29216000	-0.00004000
C	1.22808000	-0.36977000	0.00002000
C	1.20911000	-1.78009000	0.00004000
H	2.13945000	-2.33649000	0.00007000
C	8.81065000	3.05188000	-0.03407000
H	9.06946000	3.29551000	-1.06747000
H	9.52620000	2.33571000	0.36820000
H	8.82101000	3.95512000	0.57639000

G1XBme²⁺

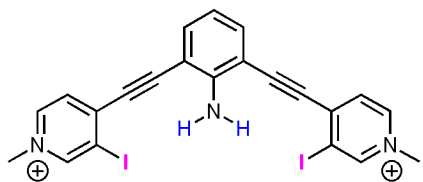


Coordinates for G1XBme²⁺:

2	1			
I	-3.57334000	-1.91367000	-0.01268000	
I	3.57324000	-1.91422000	0.01247000	
N	-7.45897000	-0.08752000	-0.00240000	

N	7.45867000	-0.08825000	-0.00050000
C	-6.41298000	-0.94230000	-0.00448000
H	-6.65776000	-1.99695000	-0.00810000
C	-5.10114000	-0.49099000	-0.00356000
C	-4.84764000	0.90918000	0.00147000
C	-5.97708000	1.76583000	0.00450000
H	-5.83982000	2.84051000	0.00619000
C	-7.25310000	1.25170000	0.00303000
H	-8.13721000	1.87771000	0.00479000
C	-3.55212000	1.46364000	0.00101000
C	-2.46327000	2.01392000	0.00090000
C	-1.21722000	2.70031000	0.00070000
C	-1.20715000	4.11453000	0.00111000
H	-2.14832000	4.65403000	0.00168000
C	0.00011000	4.80945000	0.00067000
H	0.00017000	5.89438000	0.00091000
C	1.20731000	4.11441000	-0.00010000
H	2.14852000	4.65384000	-0.00046000
C	-0.00002000	1.99452000	0.00009000
H	-0.00007000	0.91042000	-0.00014000
C	1.21725000	2.70020000	-0.00028000
C	2.46323000	2.01368000	-0.00084000
C	3.55199000	1.46321000	-0.00123000
C	4.84743000	0.90856000	-0.00202000
C	5.97704000	1.76535000	-0.00623000
H	5.83968000	2.84002000	-0.00869000
C	7.25281000	1.25122000	-0.00573000
H	8.13725000	1.87688000	-0.00852000
C	5.10088000	-0.49138000	0.00297000
C	6.41291000	-0.94286000	0.00300000
H	6.65728000	-1.99755000	0.00663000
C	-8.84763000	-0.60840000	0.02872000
H	-8.84029000	-1.66254000	-0.24449000
H	-9.45199000	-0.05132000	-0.68825000
H	-9.25501000	-0.48895000	1.03542000
C	8.84888000	-0.60544000	-0.02186000
H	9.29591000	-0.39475000	-0.99598000
H	8.83343000	-1.68024000	0.15157000
H	9.42248000	-0.11697000	0.76740000

G2XBme²⁺-no F

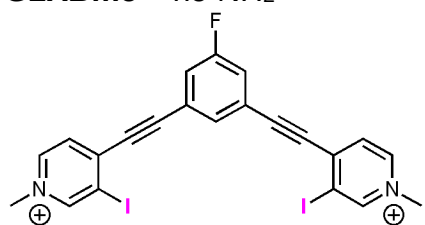


Coordinates for G2XBme²⁺-no F:

2 1			
I	3.55832000	-1.93046000	-0.00324000
H	0.00002000	5.90392000	-0.00268000
N	-0.00047000	0.61871000	0.00016000
H	0.86393000	0.10301000	0.00000000
H	-0.86497000	0.10319000	0.00003000

N	7.44721000	-0.10948000	-0.00283000
C	4.83308000	0.89476000	0.00052000
C	5.08982000	-0.50644000	-0.00038000
C	3.54410000	1.44976000	-0.00011000
C	1.22823000	2.70415000	-0.00103000
C	2.46622000	2.03030000	-0.00060000
C	6.39789000	-0.96169000	-0.00115000
H	6.64008000	-2.01693000	-0.00156000
C	-0.00033000	1.96601000	-0.00065000
C	-2.46684000	2.03072000	-0.00051000
C	1.19996000	4.11517000	-0.00173000
H	2.14479000	4.64884000	-0.00200000
C	-1.22876000	2.70438000	-0.00099000
C	-3.54478000	1.45031000	-0.00006000
C	-0.00008000	4.81996000	-0.00210000
C	5.96852000	1.74869000	-0.00028000
H	5.83424000	2.82370000	-0.00167000
C	7.24125000	1.23144000	-0.00141000
H	8.12638000	1.85611000	-0.00244000
C	-1.20025000	4.11539000	-0.00170000
H	-2.14497000	4.64923000	-0.00194000
N	-7.44736000	-0.11029000	-0.00315000
C	-4.83358000	0.89489000	0.00049000
C	-7.24188000	1.23068000	-0.00168000
H	-8.12720000	1.85507000	-0.00281000
C	-5.96932000	1.74839000	-0.00043000
C	8.83497000	-0.63017000	0.02560000
H	9.26070000	-0.47133000	1.01918000
H	9.42809000	-0.10416000	-0.72388000
H	8.82262000	-1.69460000	-0.20408000
C	-5.08982000	-0.50643000	-0.00044000
C	-6.39770000	-0.96213000	-0.00132000
H	-6.63955000	-2.01746000	-0.00174000
C	-8.83473000	-0.63195000	0.02644000
H	-9.25586000	-0.48393000	1.02368000
H	-8.82301000	-1.69383000	-0.21487000
H	-9.43160000	-0.09824000	-0.71451000
I	-3.55775000	-1.92984000	-0.00327000
H	-5.83544000	2.82345000	-0.00188000

G2XBme²⁺-no NH₂



Coordinates for G2XBme²⁺-no NH₂:

2 1

I	3.60588000	-2.10022000	-0.00426000
F	0.00006000	5.93061000	-0.00351000
H	-0.00003000	0.71808000	0.00034000
N	7.47534000	-0.24067000	-0.00122000
C	4.85698000	0.73286000	0.00126000
C	5.12104000	-0.66455000	-0.00026000
C	3.55586000	1.27789000	0.00032000
C	1.21737000	2.50832000	-0.00093000
C	2.46573000	1.82394000	-0.00030000
C	6.43745000	-1.10453000	-0.00074000
H	6.69130000	-2.15703000	-0.00178000
C	-0.00001000	1.80152000	-0.00045000
C	-2.46575000	1.82402000	-0.00036000
C	1.21672000	3.92025000	-0.00195000
H	2.14192000	4.48496000	-0.00233000
C	-1.21736000	2.50836000	-0.00096000
C	-3.55586000	1.27795000	0.00024000
C	0.00003000	4.58862000	-0.00250000
C	5.97783000	1.59983000	0.00155000
H	5.83127000	2.67331000	0.00082000
C	7.25854000	1.09667000	0.00073000
H	8.13738000	1.73013000	0.00045000
C	-1.21667000	3.92029000	-0.00198000
H	-2.14186000	4.48503000	-0.00240000
N	-7.47537000	-0.24055000	-0.00149000
C	-4.85699000	0.73294000	0.00118000
C	-7.25857000	1.09675000	0.00028000
H	-8.13735000	1.73026000	-0.00025000
C	-5.97781000	1.59990000	0.00117000
C	8.86958000	-0.74792000	0.02622000
H	9.29192000	-0.58492000	1.02045000
H	9.45641000	-0.21401000	-0.72246000
H	8.86753000	-1.81209000	-0.20447000
C	-5.12107000	-0.66450000	-0.00012000
C	-6.43746000	-1.10445000	-0.00068000
H	-6.69137000	-2.15693000	-0.00157000
C	-8.86943000	-0.74824000	0.02708000
H	-9.28733000	-0.59566000	1.02487000
H	-8.86835000	-1.80992000	-0.21488000
H	-9.45966000	-0.20663000	-0.71328000
I	-3.60591000	-2.10017000	-0.00378000
H	-5.83126000	2.67338000	0.00018000

The electrostatic potential surface maps shown in **Figure 4** were generated by using this geometry of the receptor to carry out a single-point energy calculation as prescribed above.

The interaction energy was computed as the difference in energy between the complex and the sum of the energies of the individual components (equation below) and were corrected for basis set superposition error (BSSE) by the counterpoise technique.⁴

$$\text{Interaction energy } (E_{\text{int}}) = E(\text{AB}) - E(\text{A}) - E(\text{B})$$

*Where $E(\text{AB})$ = Energy of Host-Guest Complex. $E(\text{A})$ = Energy of the Host. $E(\text{B})$ = Energy of Bromide.

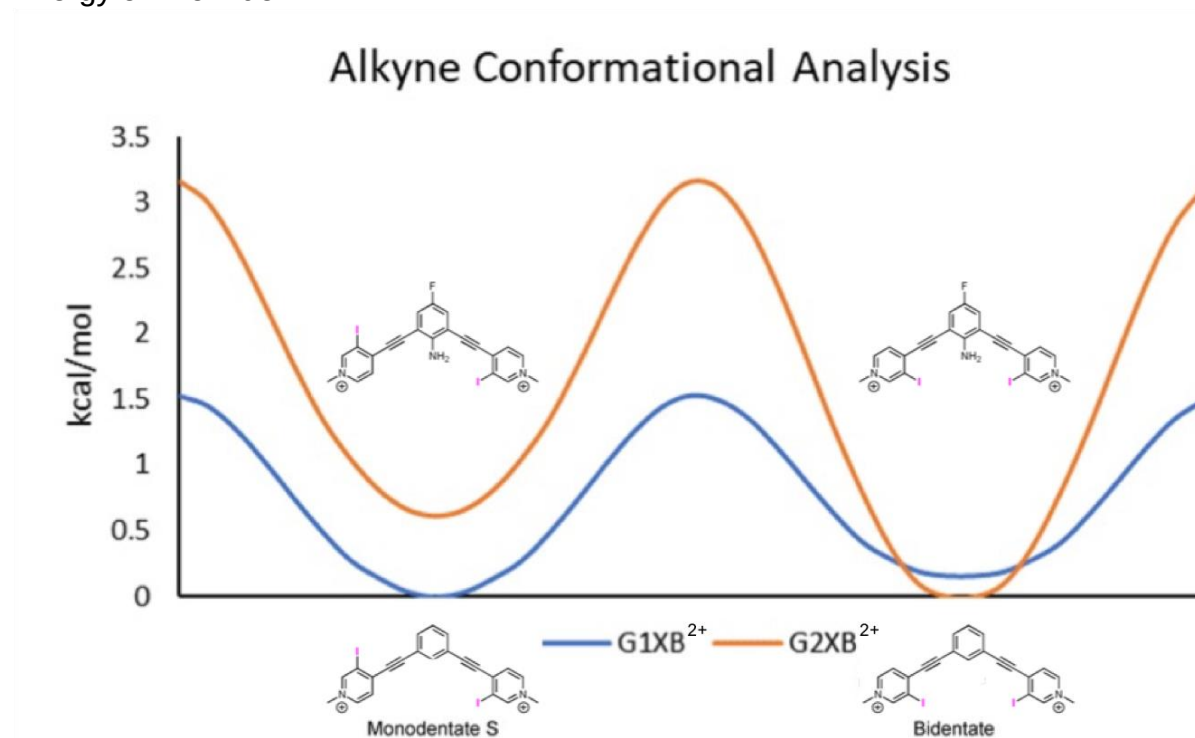


Figure S26. Conformational analysis about the alkyne bond of **G2XBme²⁺** and **G1XBme²⁺**.

Single Crystal X-ray Diffraction

X-ray diffraction data for **G1XBme²⁺•2Cl⁻**, **G1XBme²⁺•2Br⁻**, **G1XBme²⁺•2I⁻**, **G2XBme²⁺•2OTf⁻**, **G2XBme²⁺•2Br⁻**, and **G2XB²⁺•2I⁻** were collected at 100 K, while data for, **G1XBme²⁺•2OTf⁻**, were collected at 150 K. Data sets were collected on a Bruker D8 Venture using MoK α -radiation ($\lambda=0.71073$ Å) and have been corrected for absorption using SADABS⁵ area detector absorption correction program. Using Olex2⁶, the structures were solved with the SHELXT⁷ structure solution program using Direct Methods and refined with the SHELXL⁸ refinement package using least squares minimization. All non-hydrogen atoms were refined with anisotropic thermal parameters. Hydrogen atoms attached to heteroatoms were found from the residual density maps, placed, and refined with isotropic thermal parameters, unless noted below. All other hydrogen atoms were placed in geometrically calculated positions and refined using a riding model. Isotropic thermal parameters of the placed hydrogen atoms were fixed to 1.2 times the *U* value of the atoms they are linked to (1.5 times for methyl groups). Calculations and refinement of structures were carried out using APEX2⁹, SHELXTL¹⁰, and Olex2 software. Individual structure refinement details and crystal growth conditions are given below. Crystallographic data for all structures are presented in a table below..

CCDC number	1825327	1825329	1825325	1825331	1825328	1825330	1825326
Identification code	G1XBme²⁺•2Cl⁻	G1XBme²⁺•2Br⁻	G1XBme²⁺•2I⁻	G1XBme²⁺•2OTf⁻	G2XBme²⁺•2OTf⁻	G2XBme²⁺•2Br⁻	G2XB²⁺•2I⁻
Empirical formula	C ₂₂ H ₁₆ Cl ₂ I ₂ N ₂	C ₂₃ H ₂₀ Br ₂ I ₂ N ₂ O	C ₂₃ H ₂₀ I ₄ N ₂ O	C ₂₄ H ₁₆ F ₆ I ₂ N ₂ O ₆ S ₂	C ₂₄ H ₁₆ F ₇ I ₂ N ₃ O ₆ S ₂	C ₂₂ H ₁₆ Br ₂ Fl ₂ N ₃	C ₃₆ H ₄₄ Fl ₄ N ₃
Formula weight	633.07	754.03	848.01	860.31	893.32	755.00	1045.34
Temperature/K	100	100	100	150	100	100	100.0
Crystal system	monoclinic	triclinic	triclinic	orthorhombic	triclinic	monoclinic	monoclinic
Space group	<i>P</i> 2 ₁ / <i>c</i>	<i>P</i> -1	<i>P</i> -1	<i>Pbcn</i>	<i>P</i> -1	<i>P</i> 2 ₁ / <i>c</i>	<i>P</i> 2 ₁ / <i>c</i>
<i>a</i> /Å	9.1408(3)	7.2800(2)	7.3405(3)	22.337(2)	8.0582(3)	10.9739(12)	17.086(3)
<i>b</i> /Å	18.1854(6)	10.9585(4)	11.1063(4)	12.7364(13)	11.0044(4)	17.8839(19)	18.092(3)
<i>c</i> /Å	13.7305(5)	16.0936(6)	16.7600(7)	10.9081(11)	17.7067(6)	12.1266(12)	13.3174(18)
α /°	90	89.7580(10)	83.668(2)	90	99.618(2)	90	90
β /°	100.8200(10)	79.7350(10)	77.493(2)	90	91.239(2)	102.951(3)	111.458(4)
γ /°	90	78.5410(10)	78.301(2)	90	104.624(2)	90	90
Volume/Å ³	2241.83(13)	1237.53(7)	1303.08(9)	3103.2(5)	1494.58(9)	2319.4(4)	3831.4(9)
<i>Z</i>	4	2	2	4	2	4	4
ρ_{calc} /g/cm ³	1.876	2.024	2.161	1.841	1.985	2.162	1.812
Crystal size/mm ³	0.30 × 0.11 × 0.03	0.20 × 0.10 × 0.02	0.20 × 0.15 × 0.01	0.40 × 0.05 × 0.02	0.28 × 0.02 × 0.01	0.12 × 0.07 × 0.01	0.38 × 0.14 × 0.01
2 θ range for data collection/°	6.042 to 55.208	5.806 to 55.072	5.784 to 56.702	6.122 to 61.178	5.876 to 50.174	5.714 to 50.192	6.12 to 50.266
Reflections collected	37851	48110	48949	105030	44120	58944	145488
Independent reflections	5125 [<i>R</i> _{int} = 0.0383, <i>R</i> _{sigma} = 0.0242]	5654 [<i>R</i> _{int} = 0.0557, <i>R</i> _{sigma} = 0.0354]	6498 [<i>R</i> _{int} = 0.0761, <i>R</i> _{sigma} = 0.0515]	4770 [<i>R</i> _{int} = 0.0711, <i>R</i> _{sigma} = 0.0244]	5299 [<i>R</i> _{int} = 0.0515, <i>R</i> _{sigma} = 0.0274]	4112 [<i>R</i> _{int} = 0.1238, <i>R</i> _{sigma} = 0.0488]	6814 [<i>R</i> _{int} = 0.0972, <i>R</i> _{sigma} = 0.0338]
Data/restraints/parameters	5125/3/255	5654/0/278	6498/2/278	4770/0/192	5299/527/551	4112/2/281	6814/145/471
Goodness-of-fit on <i>F</i> ²	1.064	1.034	1.155	1.129	1.058	1.085	1.149
Final <i>R</i> indexes [<i>I</i> ≥ 2 σ (<i>I</i>)]	<i>R</i> ₁ = 0.0272, <i>wR</i> ₂ = 0.0591	<i>R</i> ₁ = 0.0281, <i>wR</i> ₂ = 0.0546	<i>R</i> ₁ = 0.0507, <i>wR</i> ₂ = 0.0977	<i>R</i> ₁ = 0.0383, <i>wR</i> ₂ = 0.0783	<i>R</i> ₁ = 0.0358, <i>wR</i> ₂ = 0.0836	<i>R</i> ₁ = 0.0362, <i>wR</i> ₂ = 0.0739	<i>R</i> ₁ = 0.0465, <i>wR</i> ₂ = 0.1124
Final <i>R</i> indexes [all data]	<i>R</i> ₁ = 0.0398, <i>wR</i> ₂ = 0.0634	<i>R</i> ₁ = 0.0473, <i>wR</i> ₂ = 0.0587	<i>R</i> ₁ = 0.0745, <i>wR</i> ₂ = 0.1044	<i>R</i> ₁ = 0.0609, <i>wR</i> ₂ = 0.0868	<i>R</i> ₁ = 0.0477, <i>wR</i> ₂ = 0.0895	<i>R</i> ₁ = 0.0610, <i>wR</i> ₂ = 0.0821	<i>R</i> ₁ = 0.0684, <i>wR</i> ₂ = 0.1247
Largest diff. peak/hole / e Å ⁻³	2.28/-0.63	1.21/-0.81	2.06/-1.09	1.20/-0.59	1.05/-0.63	1.02/-0.95	1.32/-1.54

G1XBme²⁺•2Cl⁻

Colorless plates were grown from a slow evaporation of an acetonitrile solution of **G1XBme²⁺•2OTf⁻** and TBA⁺Cl⁻.

The structure, displays a notable residual electron density peak of 2.3 e/ Å³ 1.643 Å from the C4 atom. This is attributed to a small disorder (< 3%) of the Iodine atom when the pyridinium arm is rotated over a 2-fold axis via the alkyne bond. Modeling this disorder results in a small reduction in the R1 statistic (<0.3%) however, nothing interesting or significant is gained through this process, therefore the model presented is absent of this disorder for simplicity.

G1XBme²⁺•2Br⁻

Colorless plates were grown from a vapor diffusion of diethyl ether into an acetonitrile/methanol solution of **G1XBme²⁺•2OTf⁻** and TBA⁺Br⁻.

G1XBme²⁺•2I⁻

Light yellow plates were grown via vapor diffusion of diethyl ether into an acetonitrile/methanol solution of **G1XBme²⁺•2OTf⁻** and TBA⁺I⁻.

The hydrogen atom bound to the oxygen of the methanol required both bond distance (DFIX 0.84 0.02) and 1,3 atom distance restraints (DANG 1.85 0.04) to produce a model reasonable and stable for refinement. The structure also displays several larger residual electron density peaks all <1 Å from Iodine atoms. These residual electron density peaks arrange in a symmetrical fashion around these Iodine atoms and are attributed to Fourier truncation ripples. Various absorption corrections were assessed however elimination of these effects were unsuccessful.

G1XBme²⁺•2OTf⁻

Colorless rods were grown from a vapor diffusion of diethyl ether into an acetonitrile solution of **G1XBme²⁺•2OTf⁻**.

G2XBme²⁺•2OTf⁻

Red needles were grown by slow evaporation of an acetonitrile and diethyl ether solution of **G2XBme²⁺•2OTf⁻**.

The structure displays disorder of one pyridinium ring about a 2-fold axis created by the alkyne bond. Due to this disorder both triflate anions also display disorder. The two positions of the pyridinium ring, and both triflate anions are tied to one free variable and demonstrate an approximate 50/50 disorder.

G2XBme²⁺•2Br⁻

Red orange plates were grown by slow evaporation of an ethyl acetate, methanol, and dichloromethane solution of **G2XBme²⁺•2OTf⁻** and TBA⁺Br⁻.

The hydrogen atoms bound to the amine in this structure were located from the difference map. Upon refinement, the N-H bond distance reduced to a distance that was

unreasonable. These distances were subsequently restrained using a DFIX 0.87 0.02 instruction.

G2XB²⁺·2I⁻

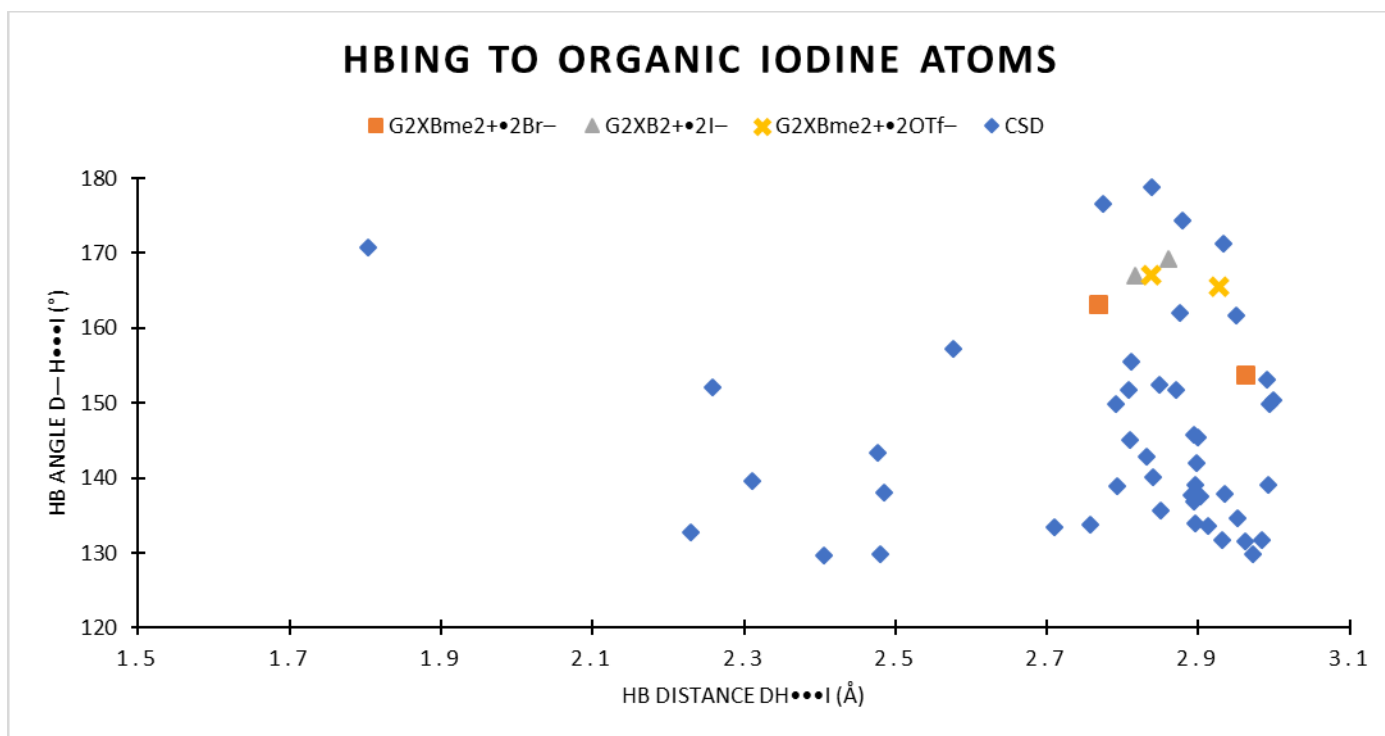
Diffraction quality crystals were grown by slow evaporation of a deuterated nitromethane, deuterated chloroform solution of **G2XB²⁺** and TBA⁺I⁻.

The hydrogen atoms bound to the amine in this structure were located from the difference map. Upon refinement, the N-H bond distance reduced to a distance that was unreasonable. These distances were subsequently restrained using a DFIX 0.87 0.02 instruction. The octyl tails of the scaffold display some disorder and have been modeled appropriately using a combination of bond distance (SADI) and thermal ellipsoid (RIGU) restraints. The structure also displays several larger residual electron density peaks all <1 Å from Iodine atoms. These residual electron density peaks arrange in a symmetrical fashion around these Iodine atoms and are attributed to Fourier truncation ripples. Various absorption corrections were assessed however elimination of these effects were unsuccessful.

Cambridge Structure Database Search and Results

ConQuest was used to collect and measure contact data from the CSD (version 5.38 updates through Nov 2016)¹¹ for HBs to organic iodine atoms. Iodine atoms were restricted to having 1 bound atom (carbon) to examine traditional organic XB donor species. HB contacts were restricted to inclusive parameters similar to those outlined by Steiner¹² which include hydrogen-acceptor distances from 0.0-3.0 Å and angles of 130.0-180.0°. Parent donor atoms were restricted to nitrogen and oxygen, while nontraditional C-H HBs were not included due to the liberal HB geometric parameters outlined. The data was limited to strictly organic structures to eliminate any possible influence by well-defined metal coordination geometries. No restrictions on disorder or R value were implemented to augment the small data set. N—H and O—H distances were normalized using the CSD methods and default values. Standard deviation is presented in parentheses following averages computed.

The above outline search returned 41 structures resulting in 46 unique contacts. Average HB distance DH...I was 2.774(0.249)Å with a HBing angle (D—H...I) of 145.781(13.378)°. A scatter plot of the findings is presented below including our HBing contacts (normalized using CSD methods and default values). Below the scatter plot is a table showing the normalized HB distances and angles of the structures reported along with the average values obtained from the CSD.



Normalized HB parameters		
Structure	HB distance	HB angle
G2XBme2+•2Br-	2.7637(5)	163.6(3)
G2XBme2+•2Br-	2.9579(5)	154.2(3)
G2XB2+•2I-	2.8126(7)	167.3(5)
G2XB2+•2I-	2.8576(8)	169.6(4)
G2XBme2+•2OTf-	2.9225(3)	166.0(2)
G2XBme2+•2OTf-	2.8330(6)	167.52(18)
CSD averages	2.7748	145.78

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