Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Simple acyclic molecules containing a single charge-assisted O–H group can recognize anions in acetonitrile:water mixtures

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Synthesis and characterization

General remarks

All chemicals (including solvents) were bought from commercial suppliers and used as received. NMR spectra were collected on Bruker Avance 400 or Bruker Avance 600 spectrometers and are referenced to the residual solvent signal.[1] Infrared spectra were recorded on a Perkin-Elmer Spectrum Two FT-IR Spectrometer fitted with an ATR Two Single Reflection Diamond. Electrospray ionisation mass spectrometry data were acquired on a Micromass Waters ZMD spectrometer.

Characterization data

1·BPh_4

Note: it was possible to obtain satisfactory ^{1}H NMR data for **1·BPh_4** in d_6-DMSO, but significant peak broadening was observed, so a spectrum recorded in CD_3CN is provided instead.

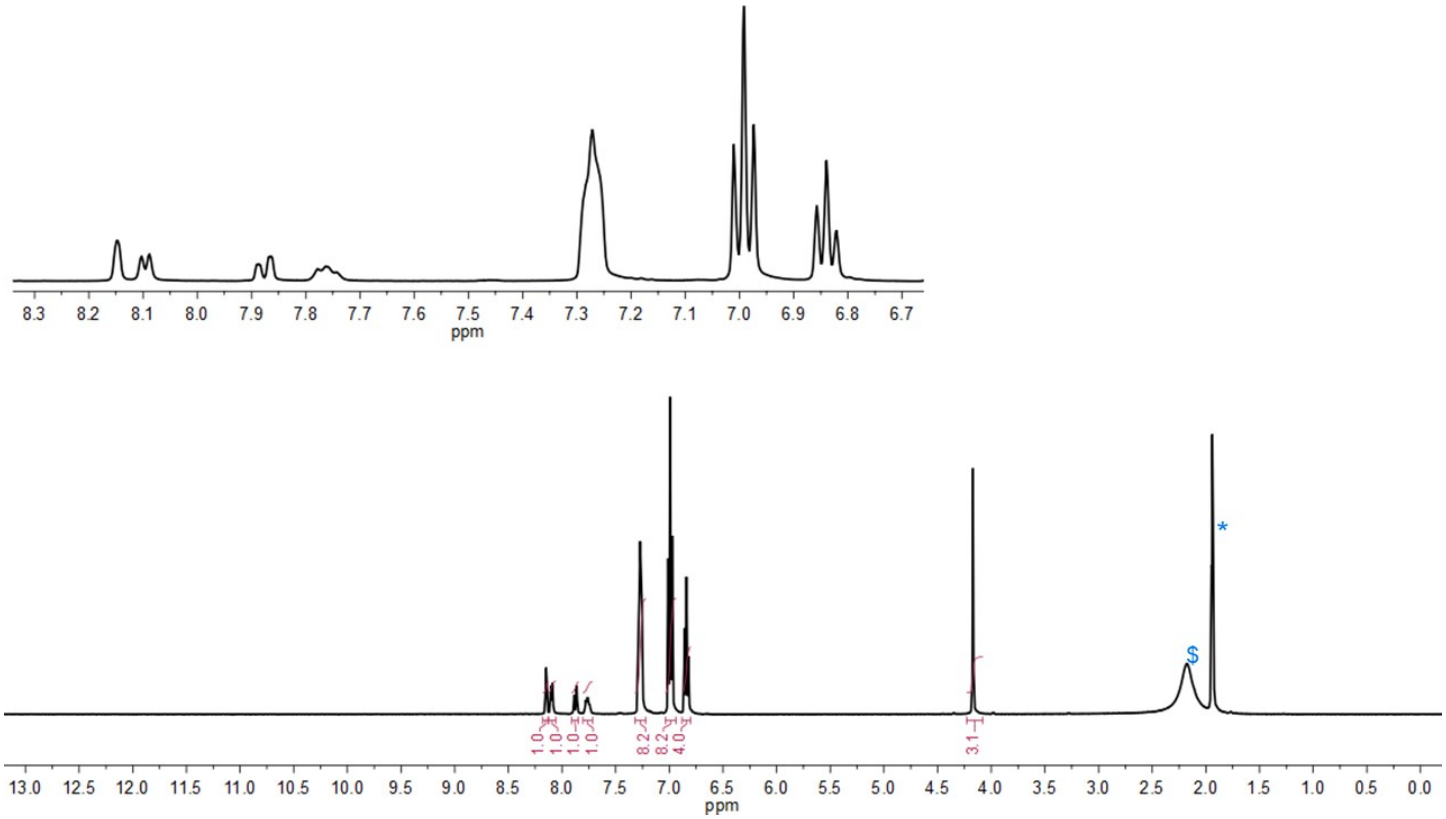

Figure S1. ^{1}H NMR spectrum of **1·BPh_4**, peak labelled * results from incompletely deuterated NMR solvent, peak labelled $ results from water (CD_3CN, 400 MHz, 298 K).

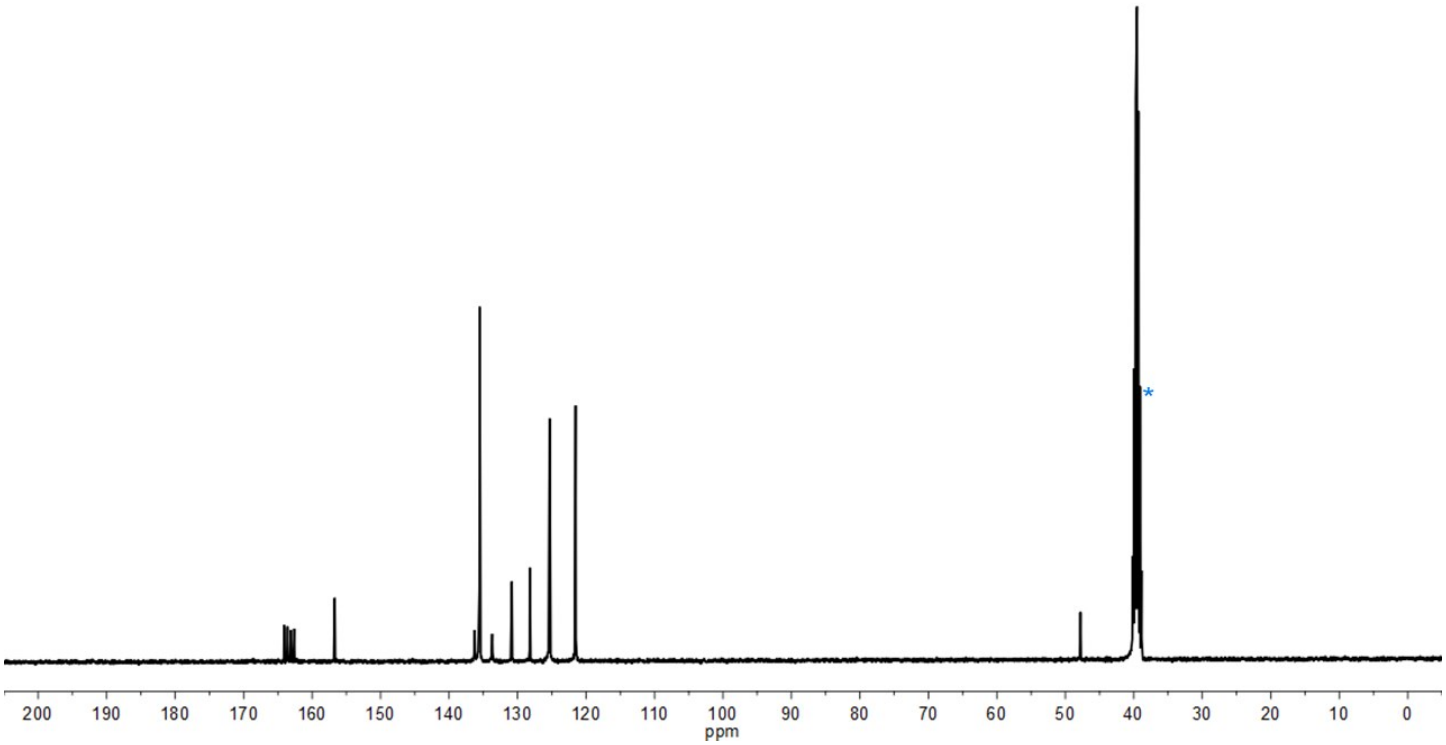

Figure S2. ^{13}C NMR spectrum of **1·BPh_4**, peak labelled * results from incompletely deuterated NMR solvent (d_6-DMSO, 101 MHz, 298 K).

2·BPh_4

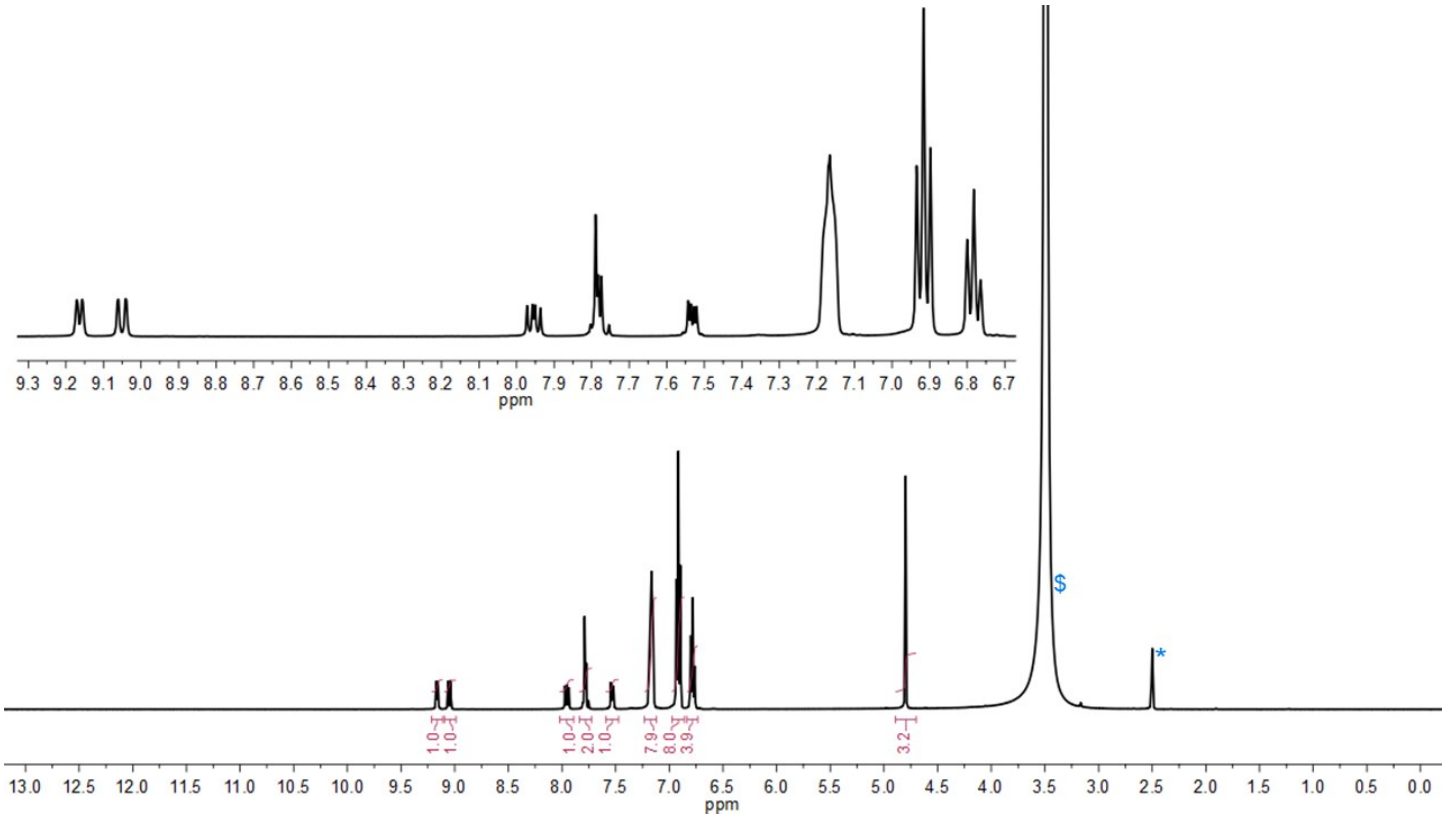

Figure S3. ^{1}H NMR spectrum of **2·BPh_4**, peak labelled * results from incompletely deuterated NMR solvent, peak labelled $ results from water (d_6-DMSO, 400 MHz, 298 K).

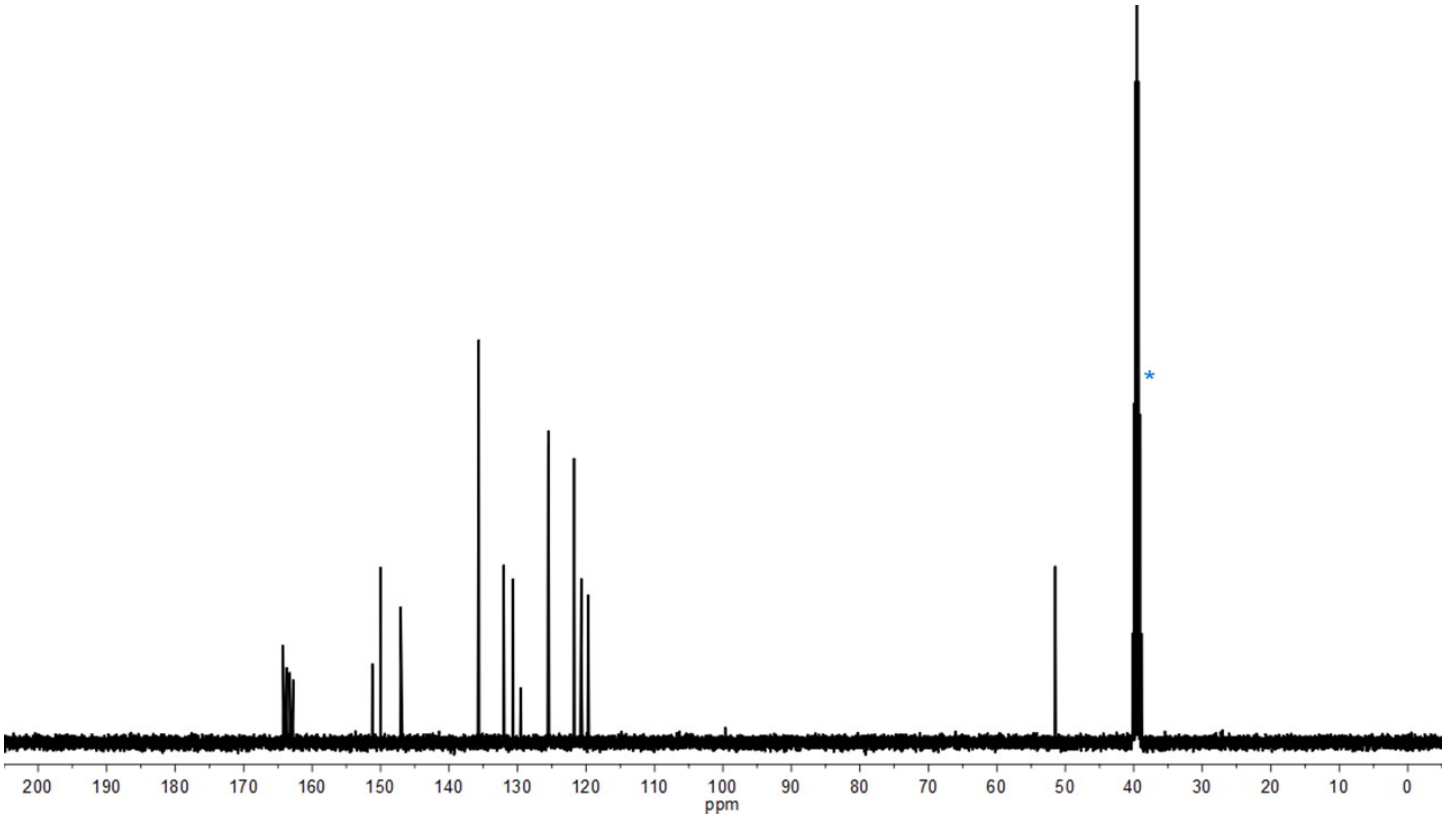

Figure S4. ^{13}C NMR spectrum of **2·BPh_4**, peak labelled * results from incompletely deuterated NMR solvent (d_6-DMSO, 101 MHz, 298 K).

2·Cl

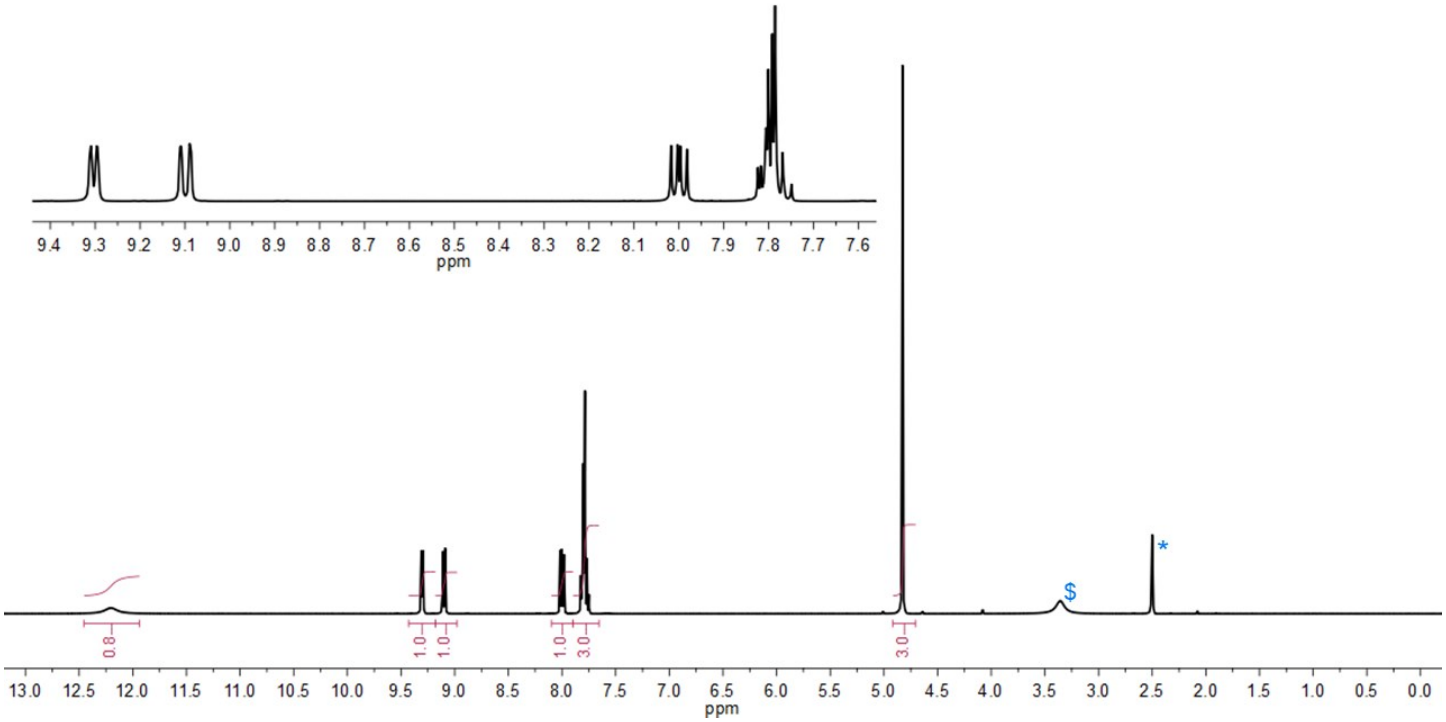

Figure S5. ^{1}H NMR spectrum of **2·Cl**, peak labelled * results from incompletely deuterated NMR solvent, peak labelled $ results from water (d_6-DMSO, 400 MHz, 298 K).

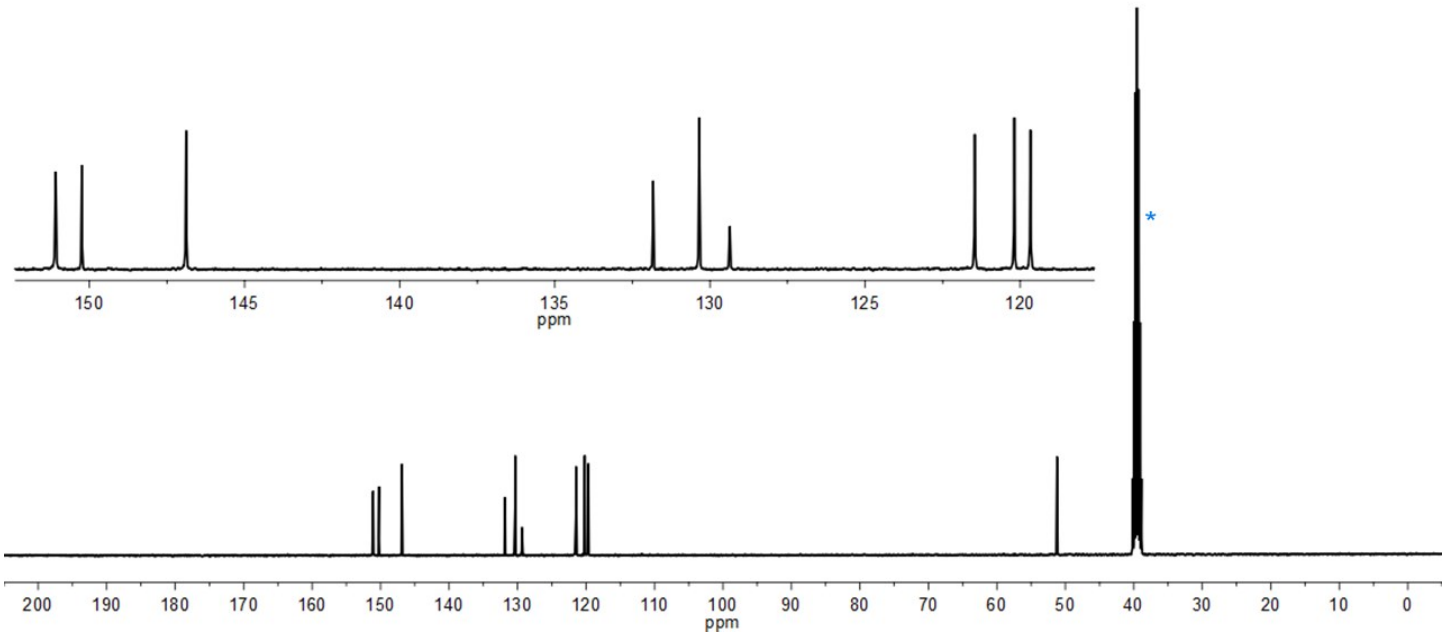

Figure S6. ^{13}C NMR spectrum of **2·Cl**, peak labelled * results from incompletely deuterated NMR solvent (d_6-DMSO, 101 MHz, 298 K).

3·Br$_2$

As described in the main text, a yellow precipitate developed in the reaction to form **3·Br$_2$**. Isolating this material by filtration, washing with acetonitrile and drying gave a material of ~ 90% purity in approximately 55% yield. The ^{1}H NMR spectrum of this material is given in Figure S7. In an effort to improve the yield of **3·Br$_2$**, we also attempted to add the bis(bromomethyl)benzene in small portions (it is not soluble enough in acetonitrile to be added dropwise as a solution) to a refluxing solution of hydroxyquinoline over several hours, but found this did not significantly affect the yield or purity of either the initial precipitate or the final product after chromatographic purification.

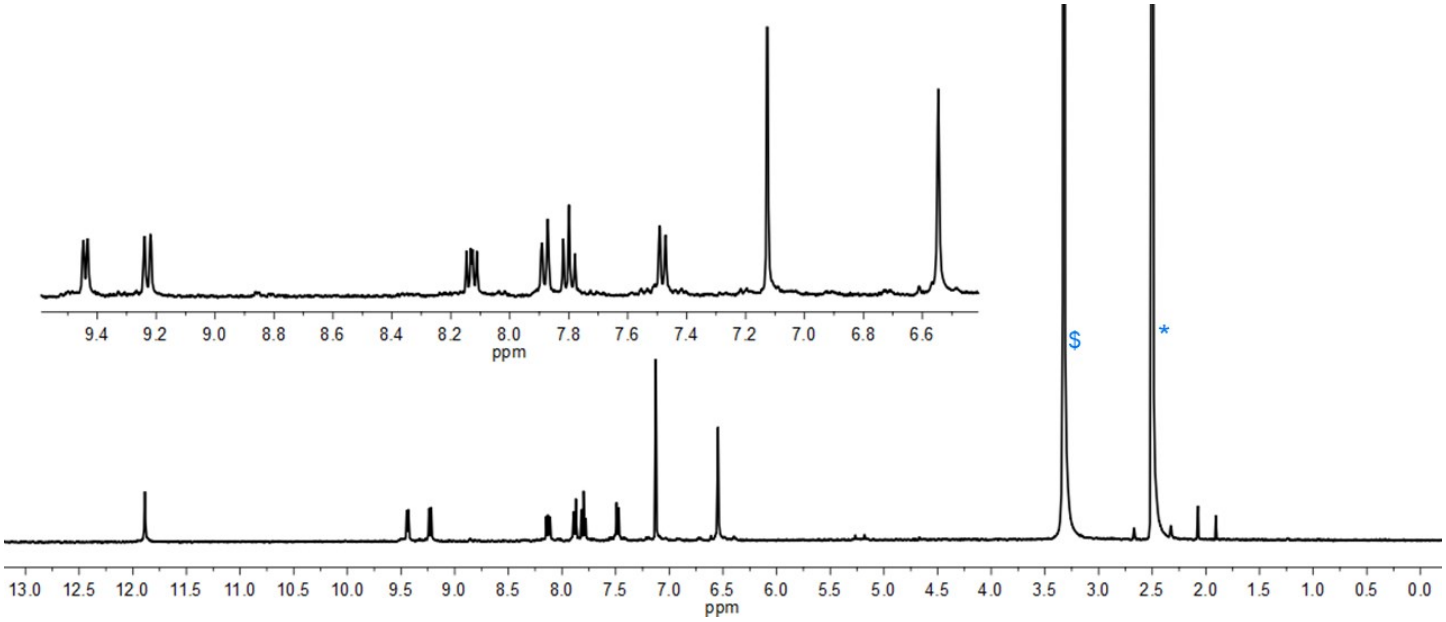

Figure S7. ^{1}H NMR spectrum of crude **3·Br$_2$**, peak labelled * results from incompletely deuterated NMR solvent, peak labelled $ results from water (d_6-DMSO, 400 MHz, 298 K).

Small quantities of **4·Br** were isolated from reactions to form **3·Br$_2$**. When a large excess of hydroxyquinoline is used, **4·Br** is a very minor by-product, however when the reaction is carried out using a small excess of hydroxyquinoline or a stoichiometric ratio (*i.e.* 1:2) then significant amounts of **4·Br** (up to 30%) form, as determined by ^{1}H NMR analysis of the crude reaction mixture. Small quantities of relatively pure **4·Br** could be isolated as yellow single crystals by filtering the yellow precipitate that developed during the reaction, and then reducing the volume of the filtrate by boiling and then allowing the mixture to cool (the ^{1}H NMR spectrum of these crystals is given in Figure S8).

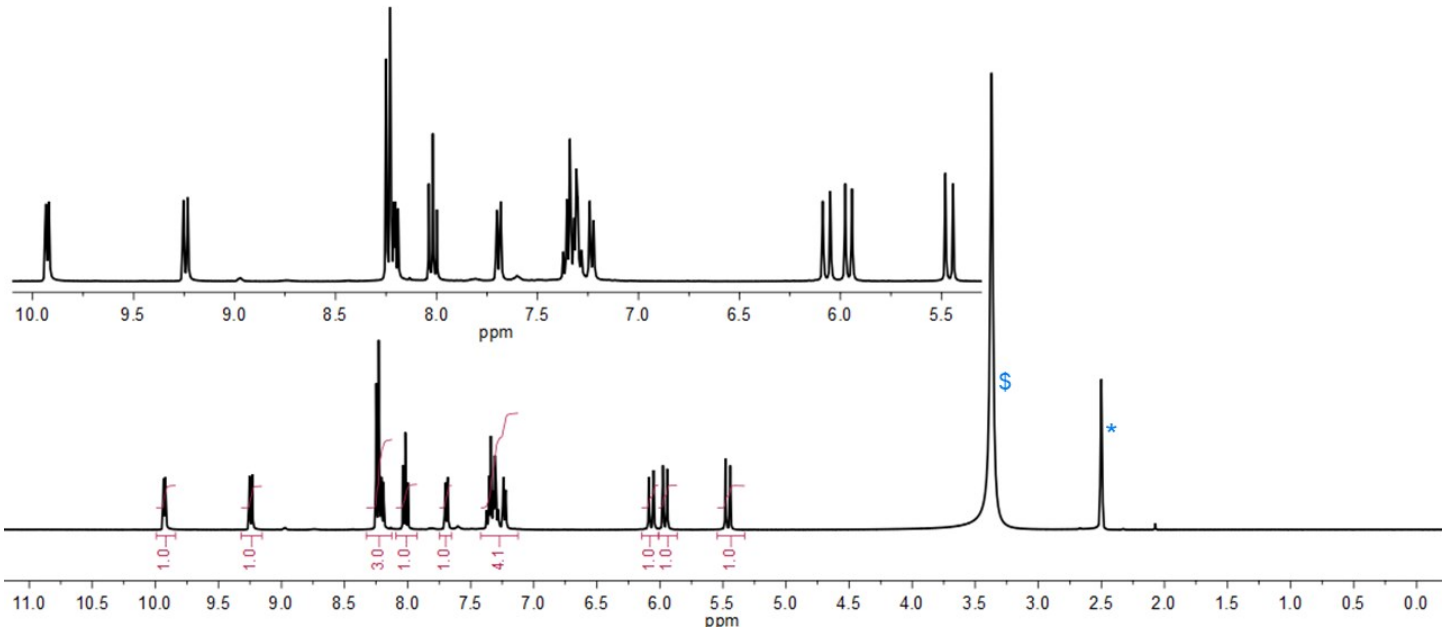

Figure S8. ^{1}H NMR spectrum of **4·Br**, peak labelled * results from incompletely deuterated NMR solvent, peak labelled $ results from water (d_6-DMSO, 400 MHz, 298 K).

Purification by column chromatography and precipitation gave pure **3·Br$_2$** in 33% overall yield (see main text). The ^{1}H and ^{13}C NMR spectra of this compound are provided in Figures S9 and S10.

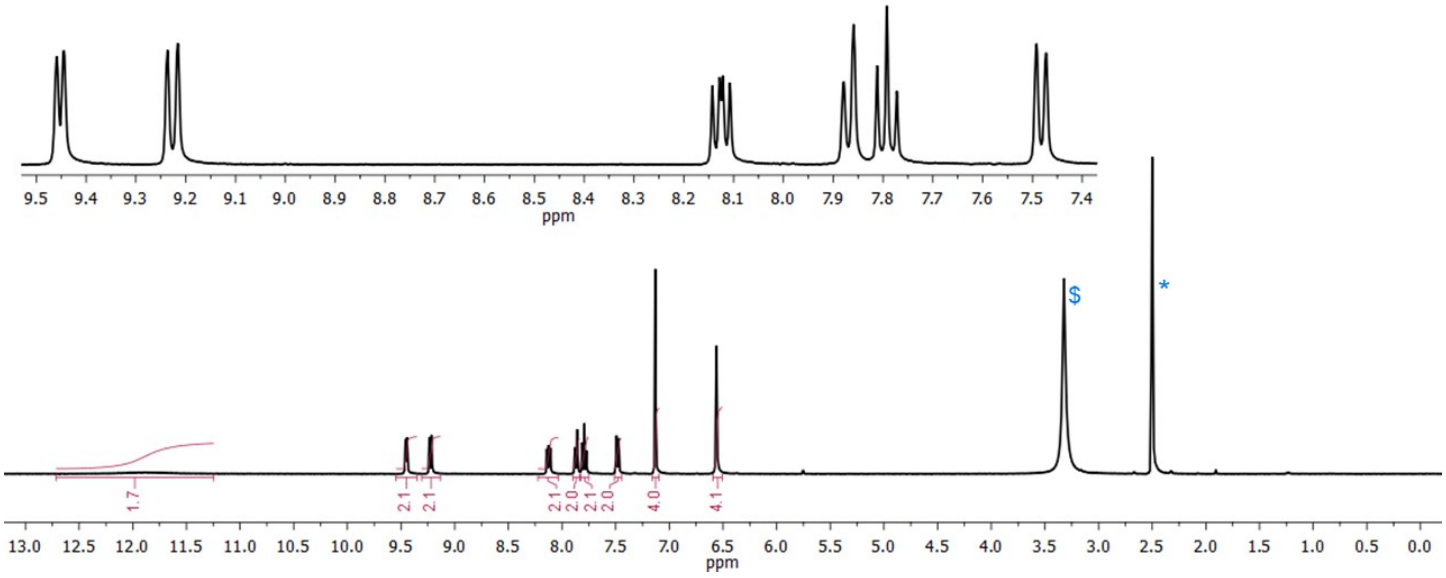

Figure S9. ^{1}H NMR spectrum of **3·Br$_2$**, peak labelled * results from incompletely deuterated NMR solvent, peak labelled $ results from water (d_6-DMSO, 400 MHz, 298 K).

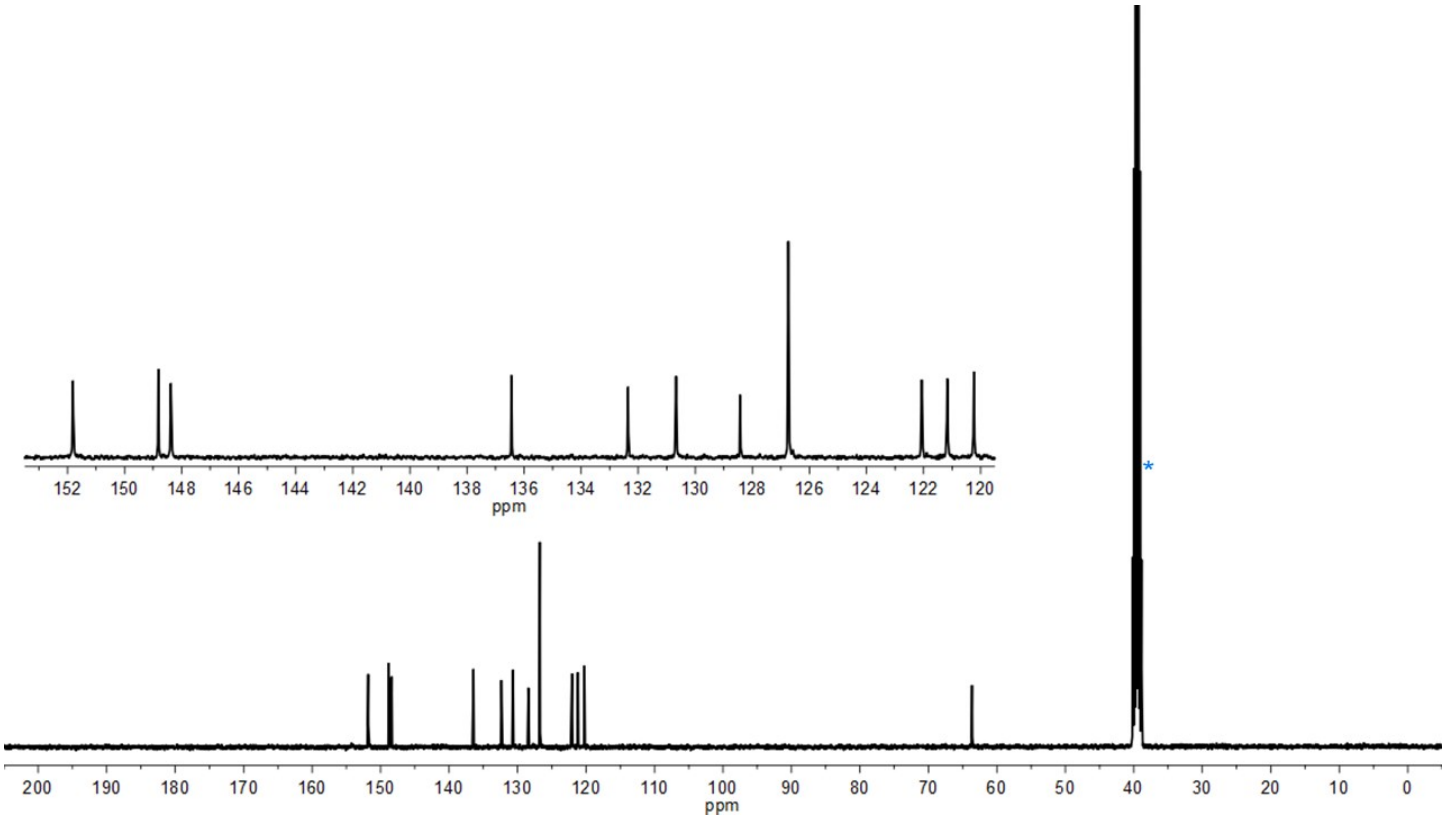

Figure S10. ^{13}C NMR spectrum of **3·Br$_2$**, peak labelled * results from incompletely deuterated NMR solvent (d_6-DMSO, 101 MHz, 298 K).

$3\cdot(PF_6)_2$

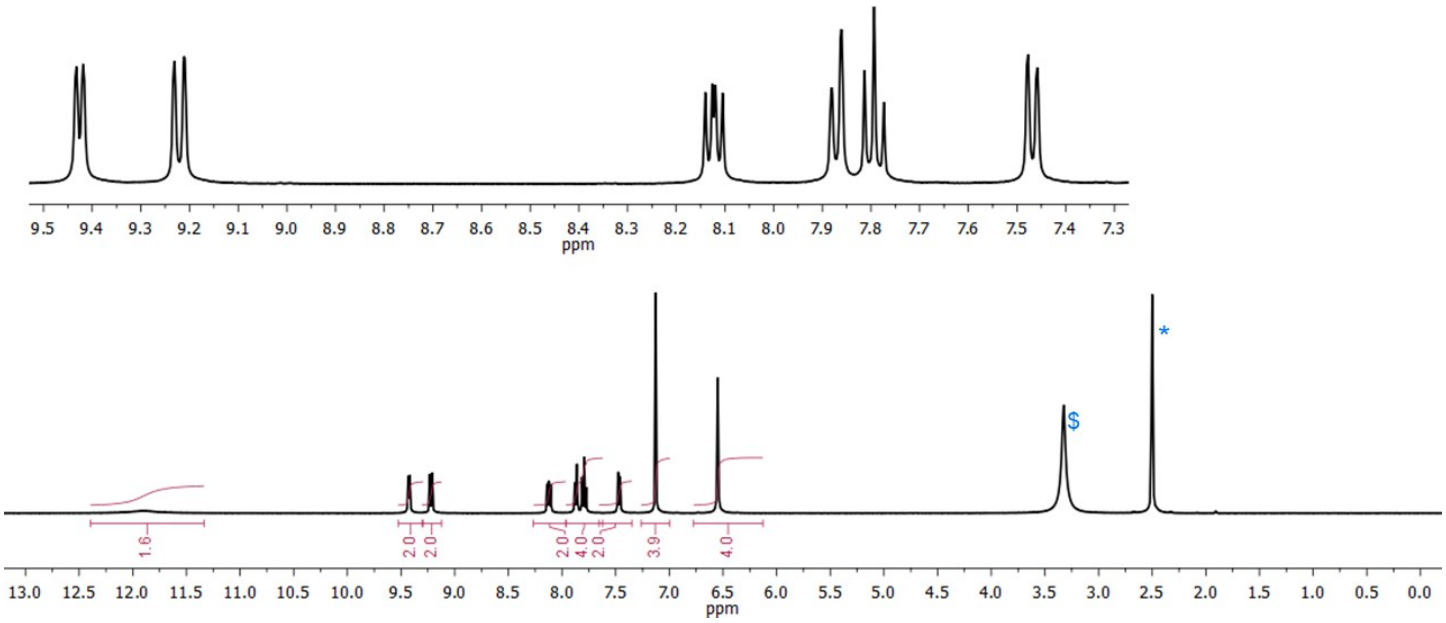

Figure S11. ^{1}H NMR spectrum of $\mathbf{3\cdot(PF_6)_2}$, peak labelled * results from incompletely deuterated NMR solvent, peak labelled $ results from water (d_6-DMSO, 400 MHz, 298 K).

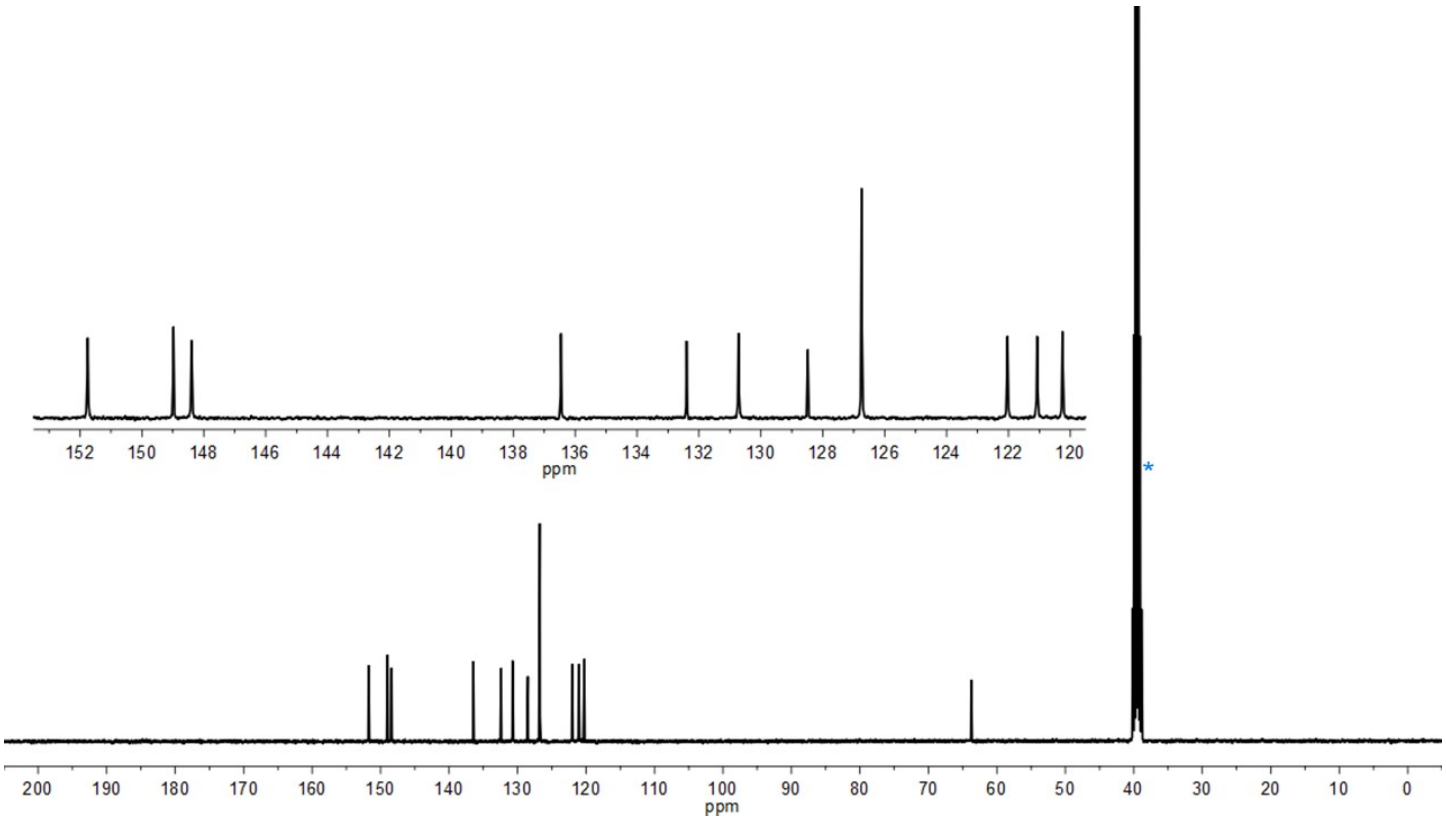

Figure S12. ^{13}C NMR spectrum of $\mathbf{3\cdot(PF_6)_2}$, peak labelled * results from incompletely deuterated NMR solvent (d_6-DMSO, 101 MHz, 298 K).

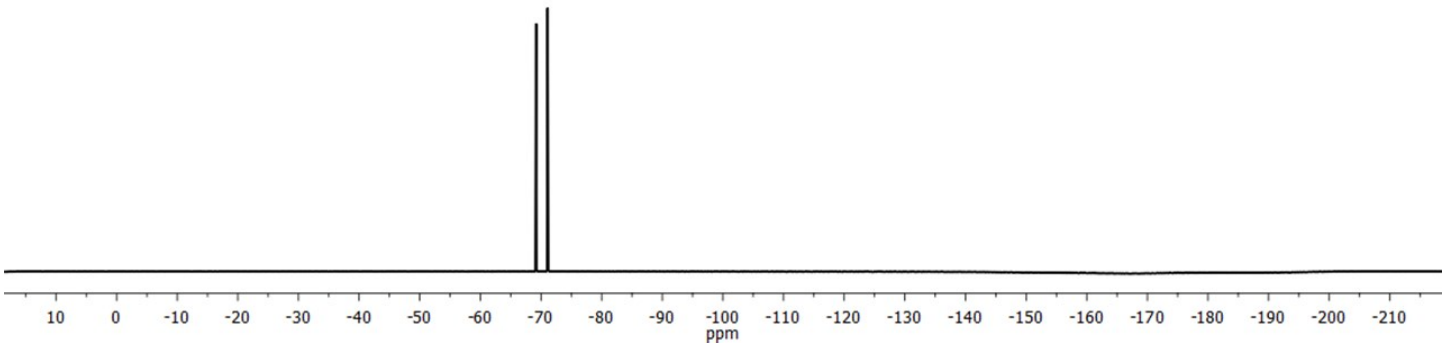

Figure S13. ^{19}F NMR spectrum of **3·$(PF_6)_2$** (d_6-DMSO, 376 MHz, 298 K).

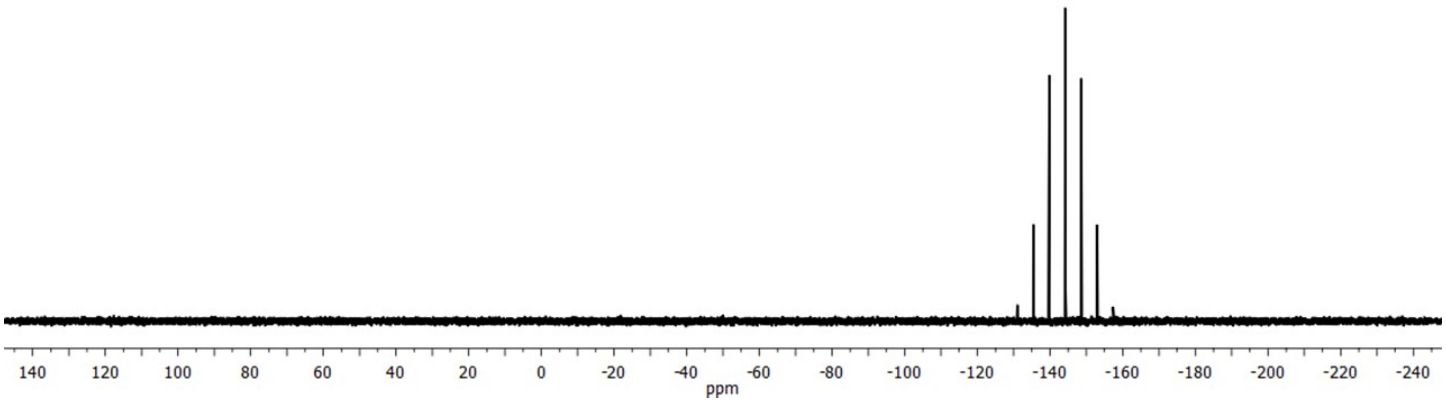

Figure S14. ^{31}P NMR spectrum of **3·$(PF_6)_2$** (d_6-DMSO, 162 MHz, 298 K).

$3^{-H}\cdot PF_6$

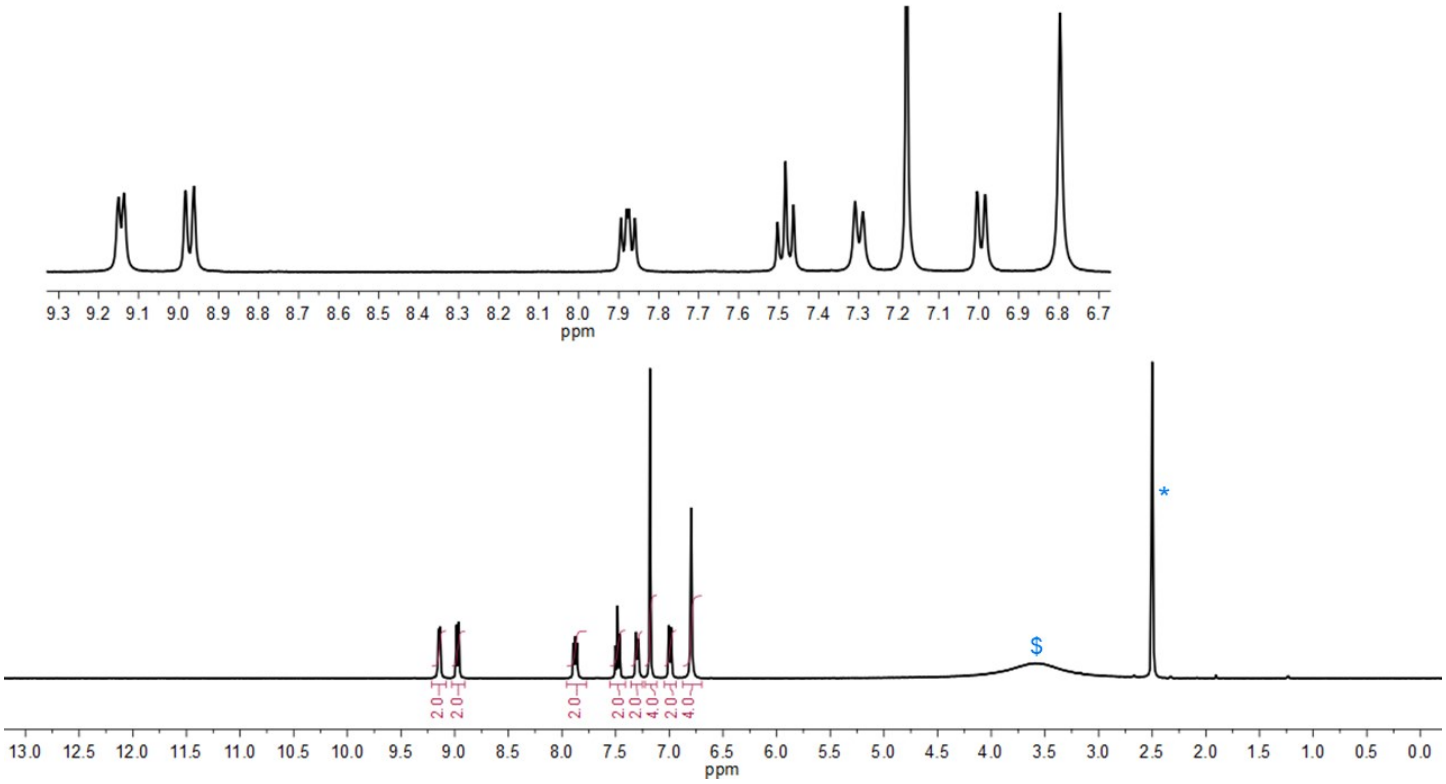

Figure S15. ^{1}H NMR spectrum of **$3^{-H}\cdot PF_6$**, peak labelled * results from incompletely deuterated NMR solvent, peak labelled $ results from water (d_6-DMSO, 400 MHz, 298 K).

The ^{13}C NMR spectrum of **$3^{-H}\cdot PF_6$** is shown in Figure S16. This compound is relatively poorly-soluble, hence the relatively low signal-to-noise ratio of the spectrum, which was recorded for an extended period of time on a saturated solution of the compound.

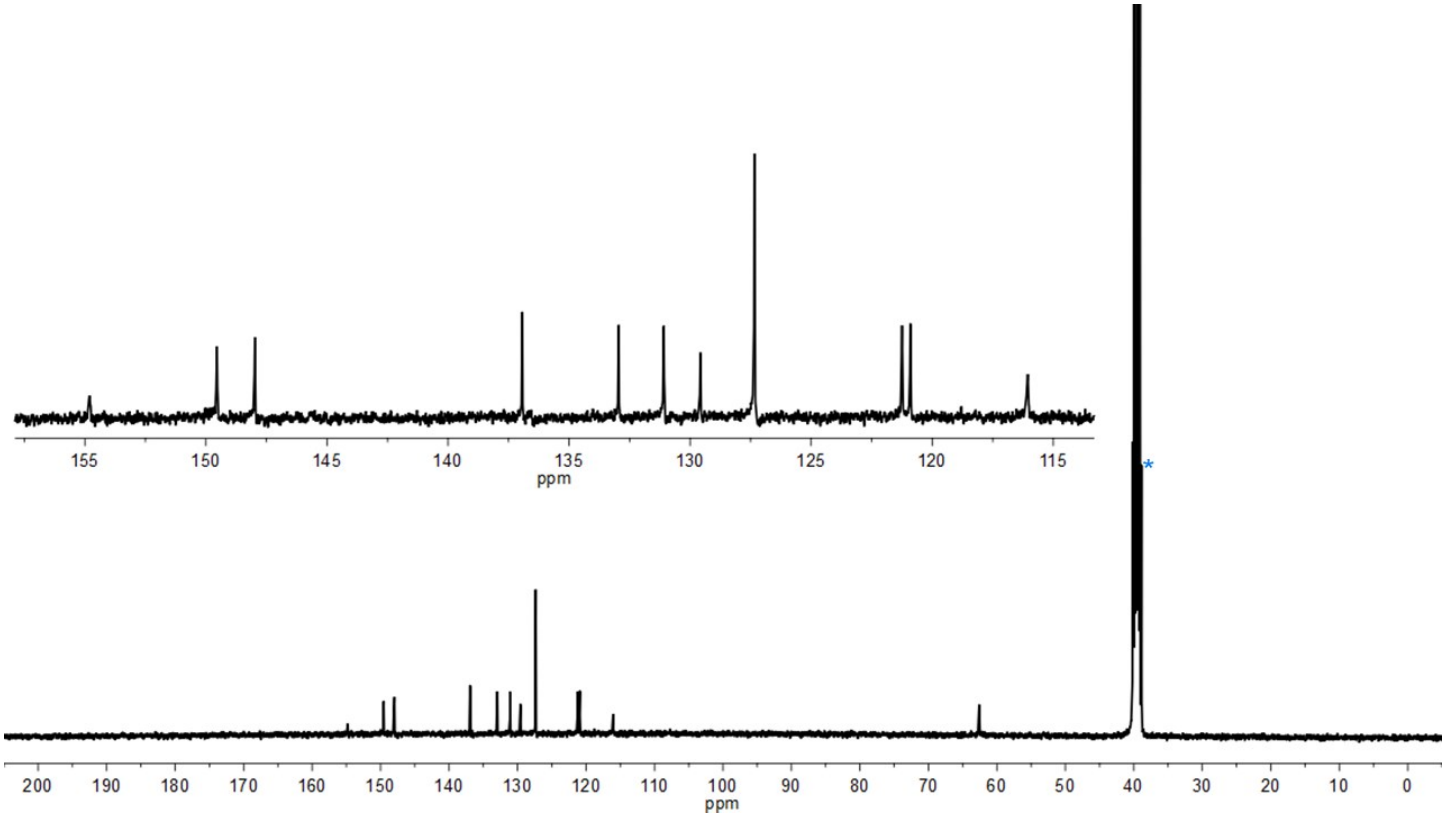

Figure S16. ^{13}C NMR spectrum of **$3^{-H}\cdot PF_6$**, peak labelled * results from incompletely deuterated NMR solvent (d_6-DMSO, 101 MHz, 298 K).

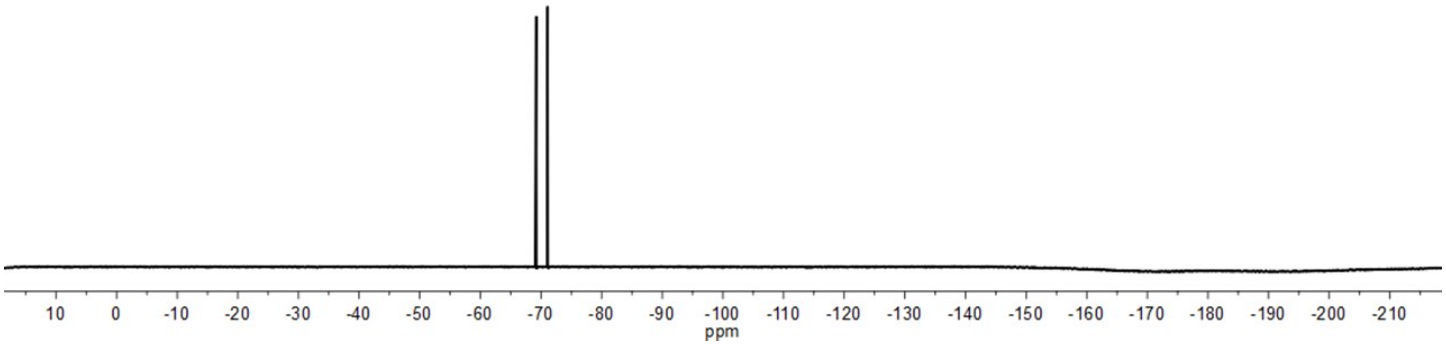

Figure S17. ^{19}F NMR spectrum of **3^{-H}·PF$_6$** (d$_6$-DMSO, 376 MHz, 298 K).

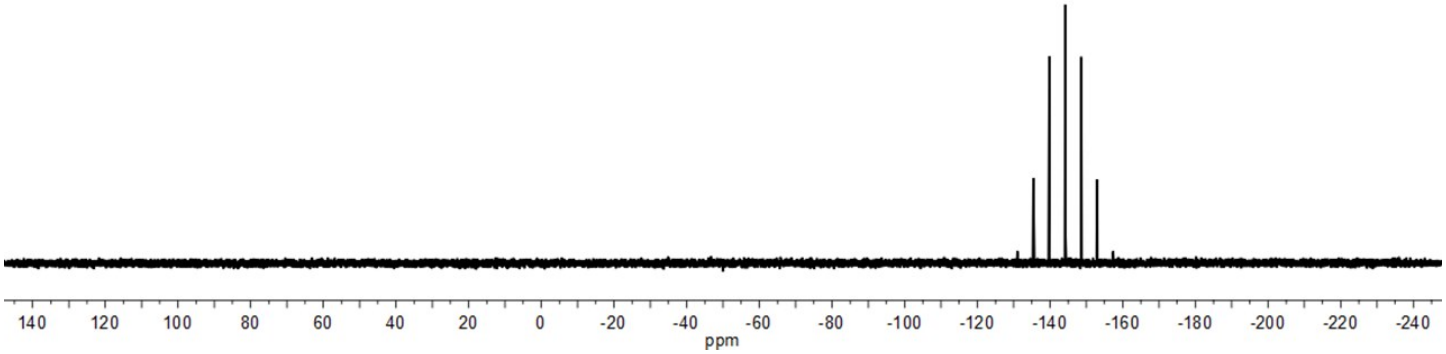

Figure S18. ^{31}P NMR spectrum of **3^{-H}·PF$_6$** (d$_6$-DMSO, 162 MHz, 298 K).

Multi-gram synthesis of 2·I

This synthesis is based on a known procedure[2] but has been optimized to give large quantities of ***2·I*** *quickly and easily.*

8-Hydroxyquinoline (5.81 g, 40.0 mmol) was dissolved in *n*-propanol (20 mL) in a heavy-walled pressure tube. Methyl iodide (3.1 mL, 7.1 g, 50 mmol) was added, the tube sealed and the solution heated to 80 °C overnight during which time it turned a deep red colour. It was cooled to room temperature, causing most of the mixture to solidify to a yellow-brown sludge. This was sonicated for 10 minutes, and then filtered to give a yellow solid. This was washed with *n*-propanol (3 × 5 mL), then diethyl ether (3 × 10 mL) and air-dried to give **2·I** as a pale yellow powder. Yield: 7.80 g (27.2 mmol, 68%).

Note: the filtrate contains a significant amount of further product (as well as a by-product), but given how inexpensive the reagents are and the ease of the reaction, it was found to be easier to repeat the reaction than attempt to isolate and purify this extra product.

^{1}H NMR (d_6-DMSO): 11.72 (s, 1H), 9.26 (d, *J* = 5.8 Hz, 1H), 9.10 (d, *J* = 8.4 Hz, 1H), 8.02 (dd, *J* = 8.4, 5.8 Hz, 1H), 7.78–7.84 (m, 2H), 7.54 (dd, *J* = 7.2, 2.0 Hz), 4.83 (s, 3H). ^{13}C NMR (d_6-DMSO): 151.2, 149.9, 146.9, 131.9, 130.5, 129.4, 121.6, 120.5, 119.5, 51.3.

NMR data (Figures S19 and S20) are consistent with those reported by Brzezinski and co-workers.[3]

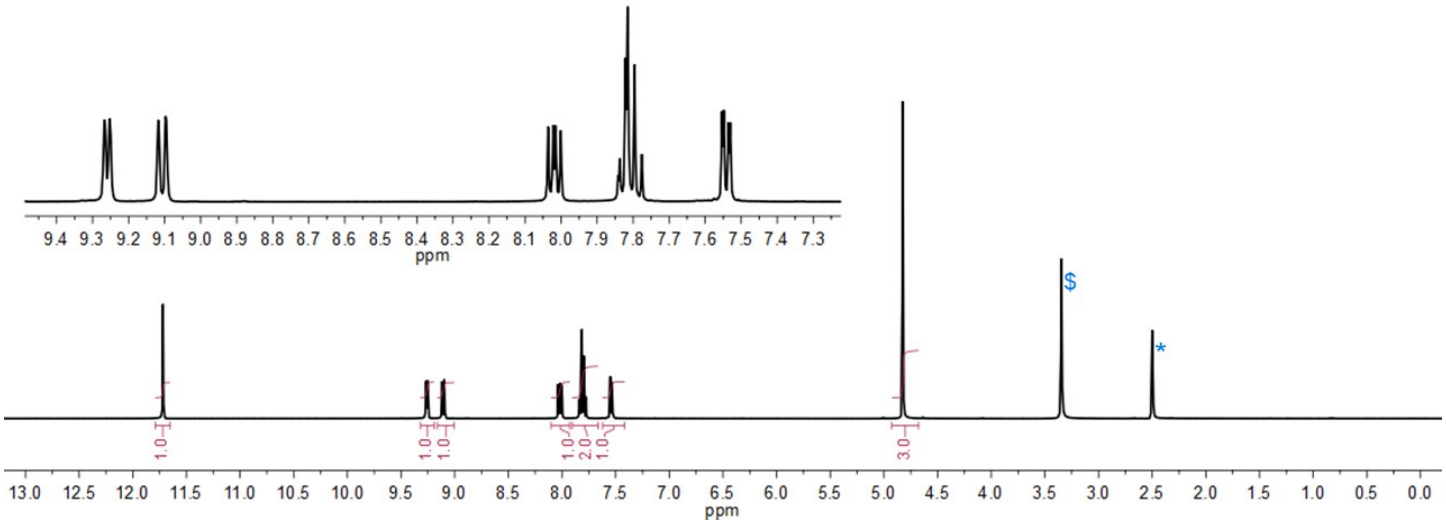

Figure S19. ^{1}H NMR spectrum of **2·I**, peak labelled * results from incompletely deuterated NMR solvent, peak labelled $ results from water (d_6-DMSO, 400 MHz, 298 K).

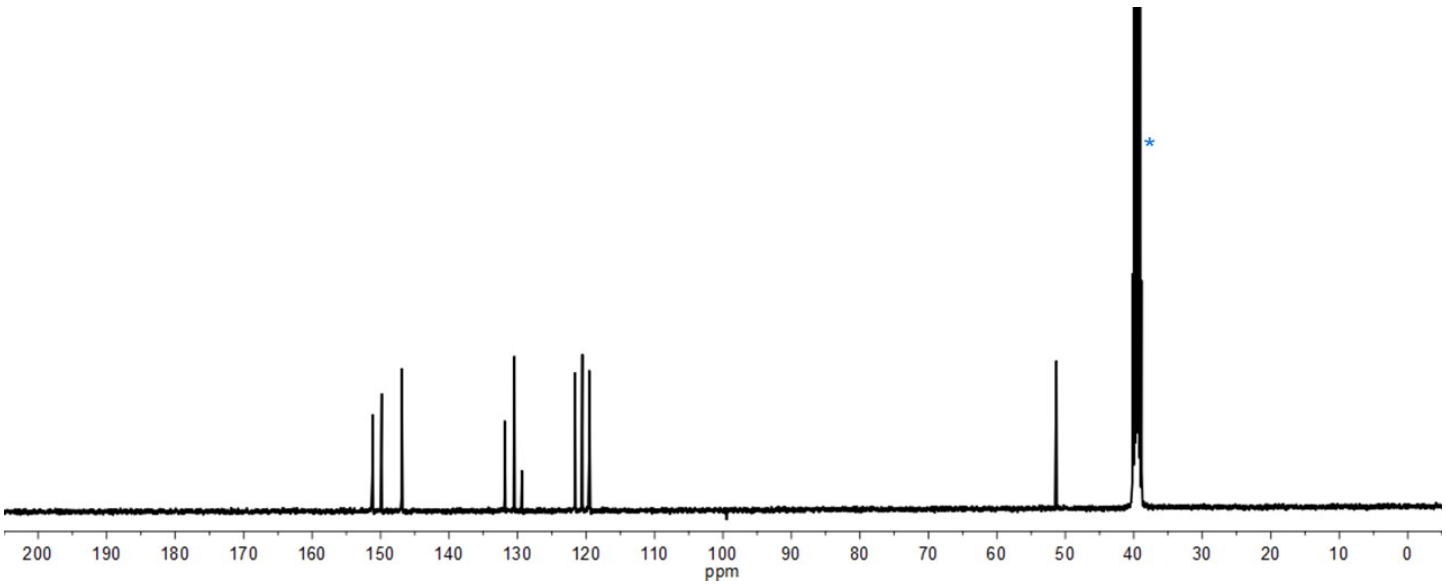

Figure S20. ^{13}C NMR spectrum of **2·I**, peak labelled * results from incompletely deuterated NMR solvent (d_6-DMSO, 101 MHz, 298 K).

$DBU^{H}{\cdot}PF_6$

1,8-Diazabicyclo[5.4.0]undec-7-ene (DBU) (0.75 mL, 0.76 g, 5.0 mmol) was dissolved in water (5 mL). $HCl_{(aq)}$ (36%, 0.50 mL, 6.0 mmol) was added resulting in the evolution of gas. A solution of NH_4PF_6 (1.6 g, 10 mmol) in water (5 mL) was added with stirring, giving white crystals. These were isolated by filtration, washed with cold water and thoroughly air-dried to give $DBU^{H}{\cdot}PF_6$. Yield: 0.80 g (54%)

^{1}H NMR (d_6-DMSO): 9.48 (br. s, 1H), 3.53–3.57 (m, 2H), 3.47 (dd, *J* = 5.8, 5.6 Hz, 2H), 3.22–3.27 (m, 2H), 2.62–2.65 (m, 2H), 2.49–2.51 (m, 2H), 1.92 (dt, *J* = 5.9, 5.8 Hz, 2H), 1.57–1.71 (m, 6H). ^{13}C NMR (d_6-DMSO): 165.4, 53.4, 47.9, 37.6, 31.7, 28.2, 25.9, 23.3, 18.8. ^{19}F NMR (d_6-DMSO): –70.2 (d, *J* = 711.3 Hz). ^{31}P NMR (d_6-DMSO): –144.2 (septet, *J* = 711.3 Hz). ESI-MS (pos.): 153.1, calc. for DBU^{H+} $[C_9H_{17}N_2]^+$ = 153.1; 451.3, calc. for $[(DBU^{H+})_2{\cdot}PF_6]^+$ $[C_{18}H_{34}N_4F_6P]^+$ = 451.2 Da. ESI-MS (neg.): 144.8, calc. for PF_6^- = 145.0 Da.

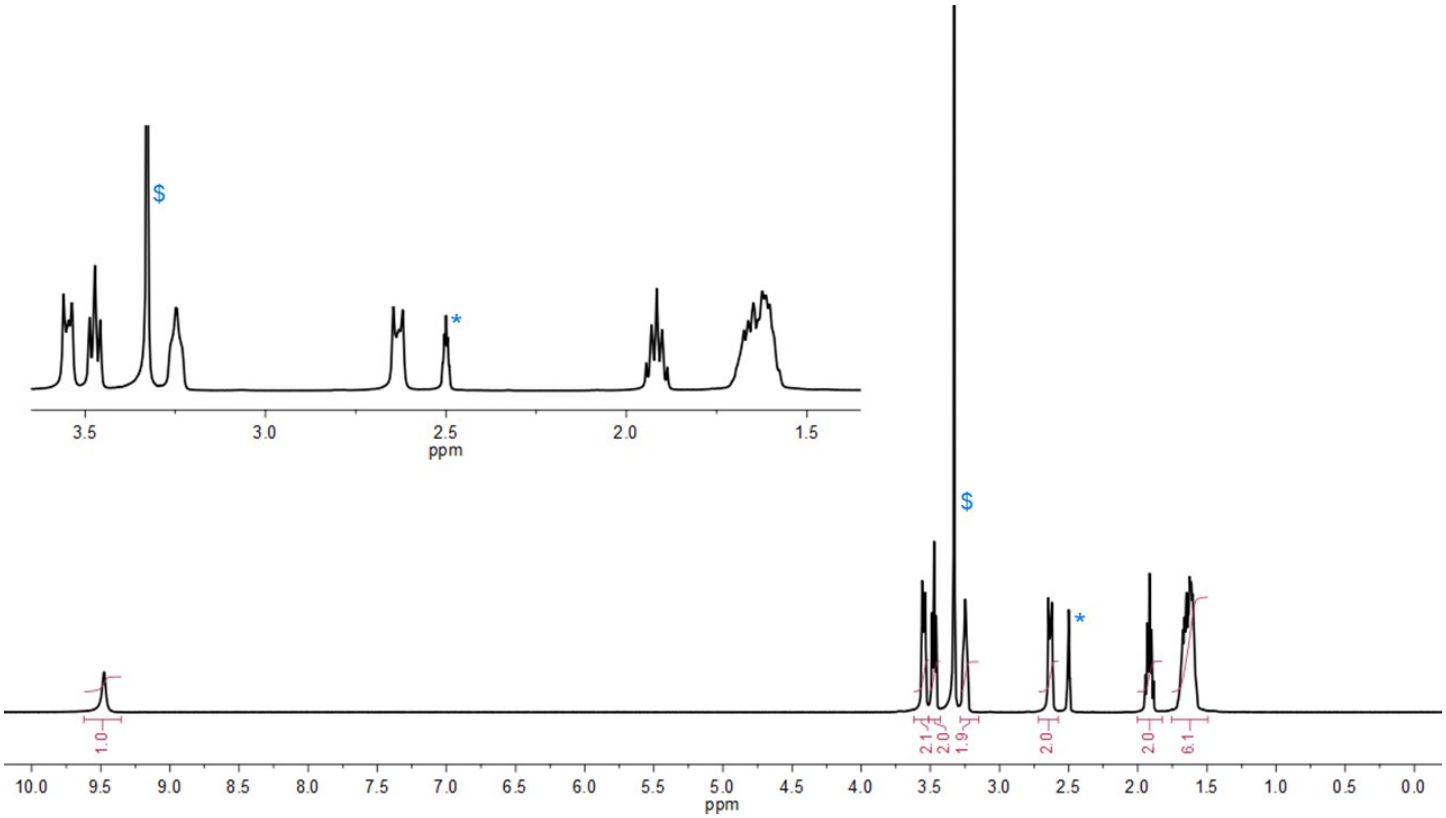

Figure S21. ^{1}H NMR spectrum of $DBU^{H}{\cdot}PF_6$, peak labelled * results from incompletely deuterated NMR solvent, peak labelled $ results from water (d_6-DMSO, 400 MHz, 298 K).

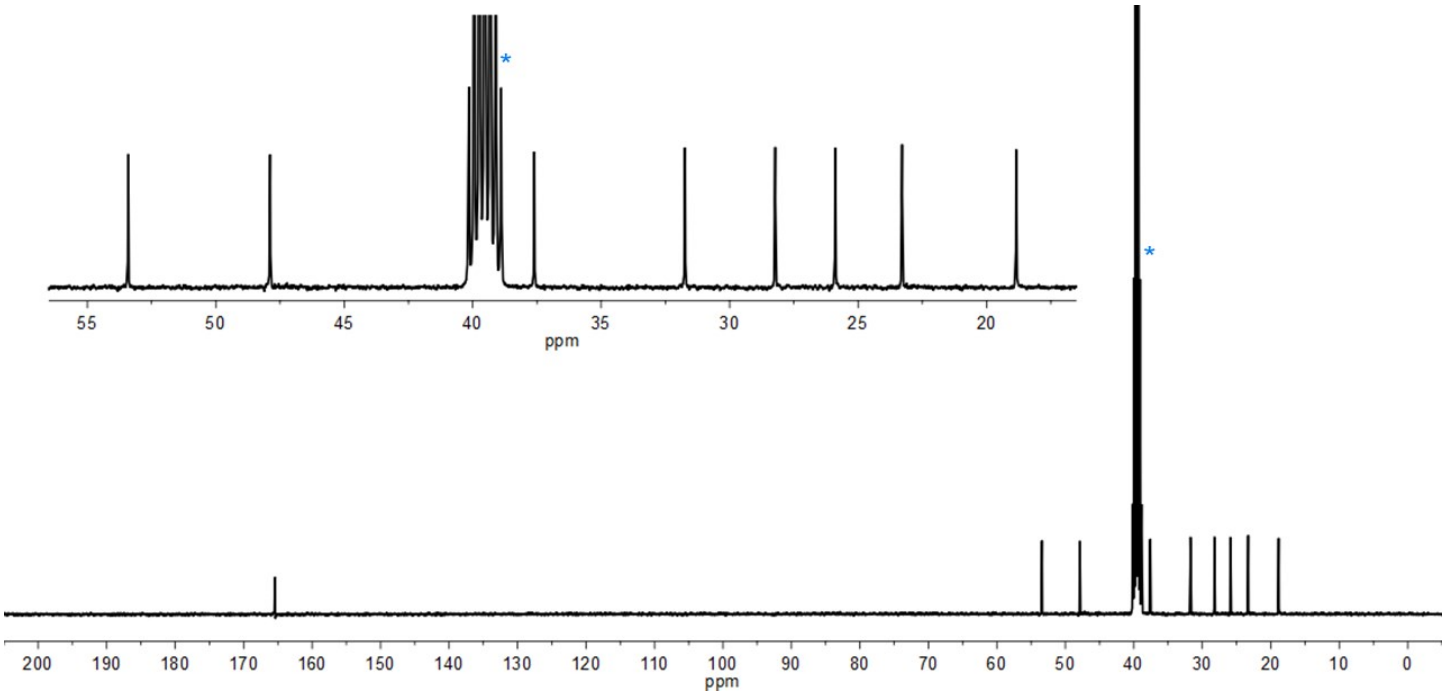

Figure S22. ^{13}C NMR spectrum of $DBU^{H}{\cdot}PF_6$, peak labelled * results from incompletely deuterated NMR solvent (d_6-DMSO, 101 MHz, 298 K).

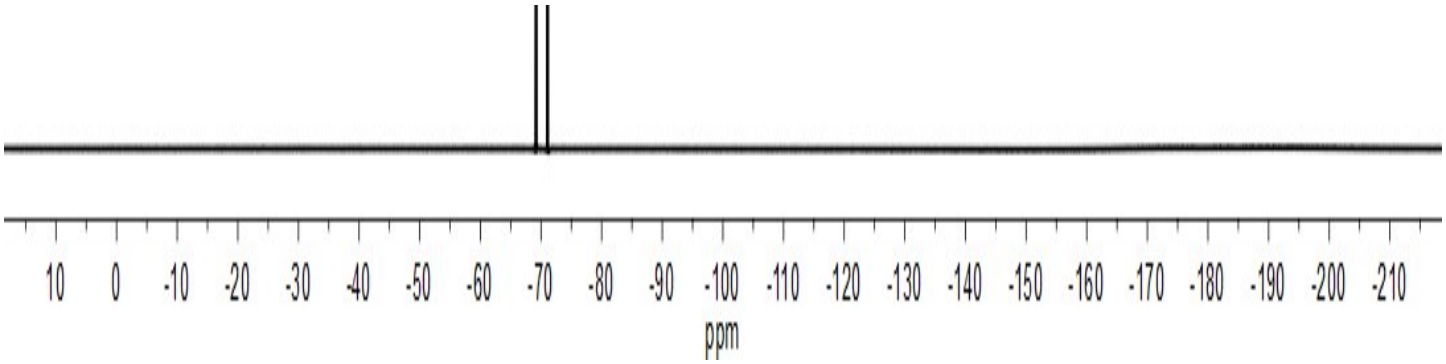

Figure S23. ^{19}F NMR spectrum of $DBU^{H}{\cdot}PF_6$ (d_6-DMSO, 376 MHz, 298 K).

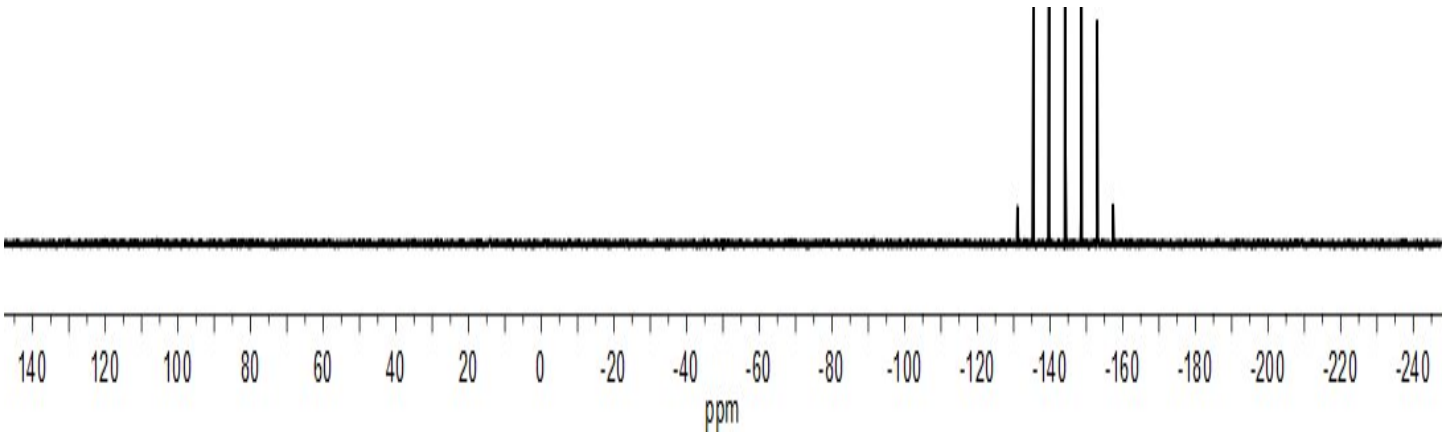

Figure S24. ^{31}P NMR spectrum of $DBU^{H}{\cdot}PF_6$ (d_6-DMSO, 162 MHz, 298 K).

Qualitative anion binding screening

A 1.0 mM solution of **2·BPh$_4$** in MeCN was prepared, and 1.0 mL aliquots of this were placed in small vials. To each of these was added one equivalent of a TBA·anion salt (10 µL of a 100 mM solution in MeCN), with the results shown in Figure S25. When I^- or HSO_4^- was added, no significant colour change was observed from the blank solution (without added anion). Addition of Cl^- caused the very pale yellow colour to become more intense, addition of $H_2PO_4^-$ caused precipitation, while addition of OAc^- caused a colour change to orange, consistent with deprotonation of **2**$^+$. Addition of SO_4^{2-} caused the solution to turn purple, and then precipitate small yellow crystals within a few minutes. Synchrotron SCXRD studies revealed that these crystals were **2$_2$·SO$_4$**.

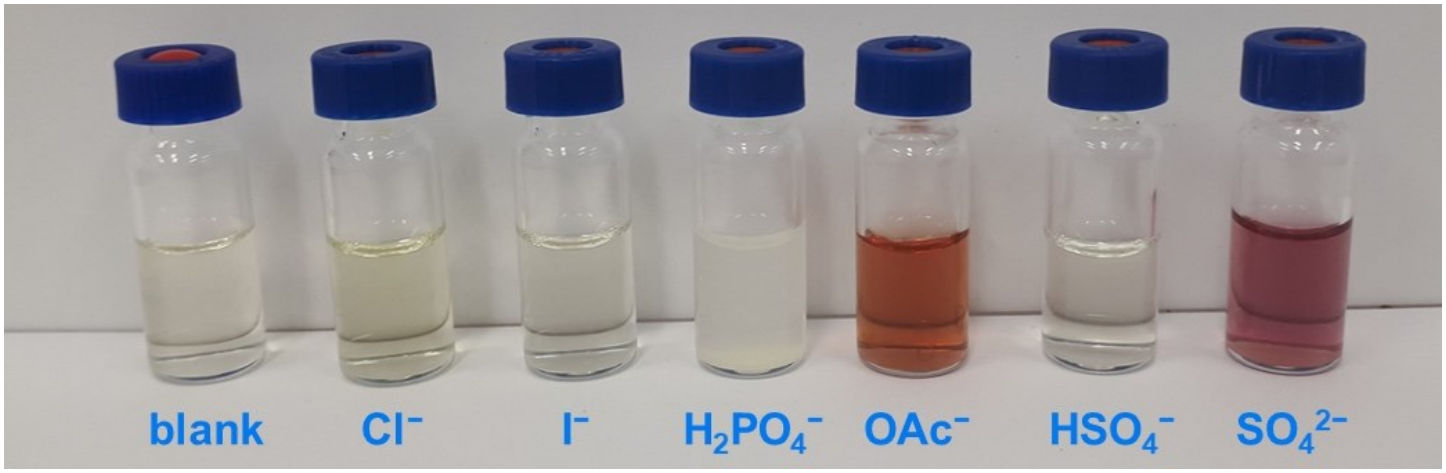

Figure S25. Photographs of 1.0 mM solutions of **2·BPh$_4$** with one equivalent of various anions as their TBA salts in MeCN.

A 1.0 mM solution of **2·BPh$_4$** in 9:1 MeCN:H_2O was prepared, and 1.0 mL aliquots of this were placed in small vials. To each of these was added one equivalent of a TBA·anion salt (10 µL of a 100 mM solution in MeCN), with the results shown in Figure S26. $H_2PO_4^-$ and HSO_4^- caused the very pale orange colour to fade, while OAc^- caused the formation of a deep orange solution, which we attribute to deprotonation of **2**$^+$.

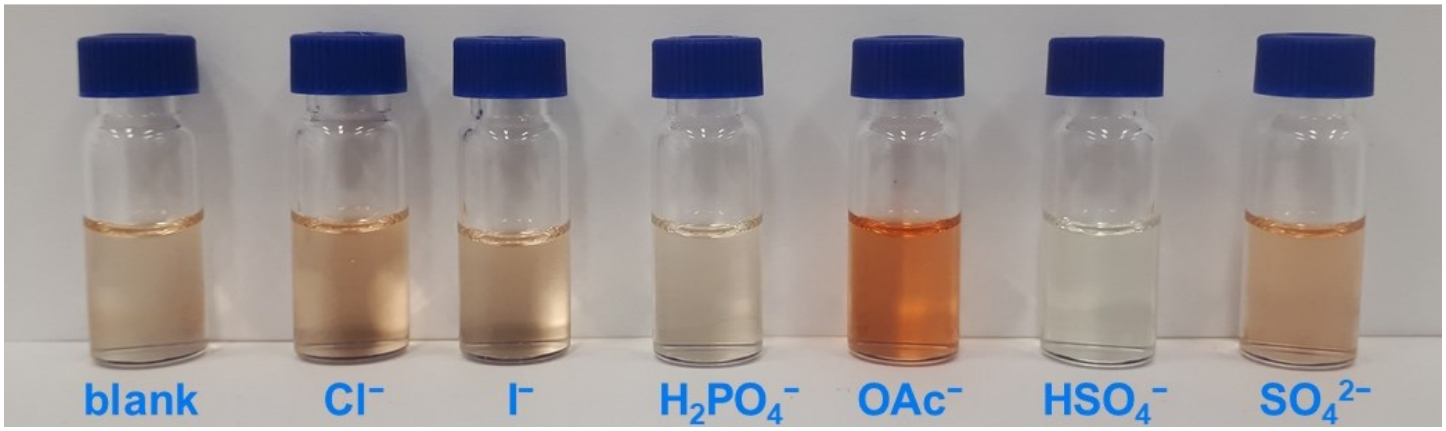

Figure S26. Photographs of 1.0 mM solutions of **2·BPh$_4$** with one equivalent of various anions as their TBA salts in 9:1 MeCN:H_2O.

A 1.0 mM solution of **3·$(PF_6)_2$** in 1:1 MeCN:MeOH was prepared, and 1.0 mL aliquots of this were placed in small vials. To each of these was added one equivalent of a TBA·anion salt (10 µL of a 100 mM solution in 1:1 MeCN: MeOH), with the results shown in Figure S27. When the anion was Cl^-, I^- or HSO_4^-, no colour change is observed from the blank solution (without added anion). Addition of $H_2PO_4^-$ causes precipitation, while addition of OAc^- causes a colour change to orange, consistent with significant deprotonation of **3^{2+}**. Addition of SO_4^{2-} causes a slight discolouration and the precipitation of small yellow crystals. Synchrotron X-ray crystallography revealed that these crystals were **3·SO_4**.

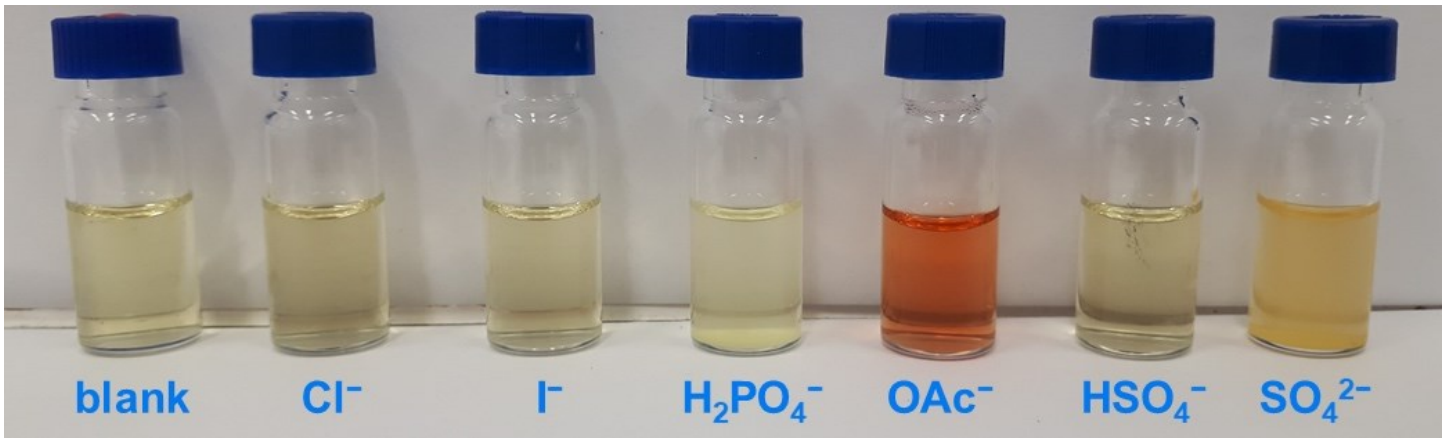

Figure S27. Photographs of 1.0 mM solutions of **3·$(PF_6)_2$** with one equivalent of various anions as their TBA salts in 1:1 MeCN:MeOH.

A 1.0 mM solution of **3^{-H}·PF_6** in 1:1 MeCN:MeOH was prepared, and 1.0 mL aliquots of this were placed in small vials. To each of these was added one equivalent of a TBA·anion salt (10 µL of a 100 mM solution in 1:1 MeCN: MeOH), with the results shown in Figure S28. Most anions do not cause a significant colour change from the blank solution (without added anion). Addition of $H_2PO_4^-$ causes a slight lightening of the colour, while addition of HSO_4^- causes a significant lightening of the colour. We attribute both of these colour changes to proton transfer from the anion to **3^{-H}·PF_6**, with this occurring to a much greater extent with the more acidic HSO_4^- anion.

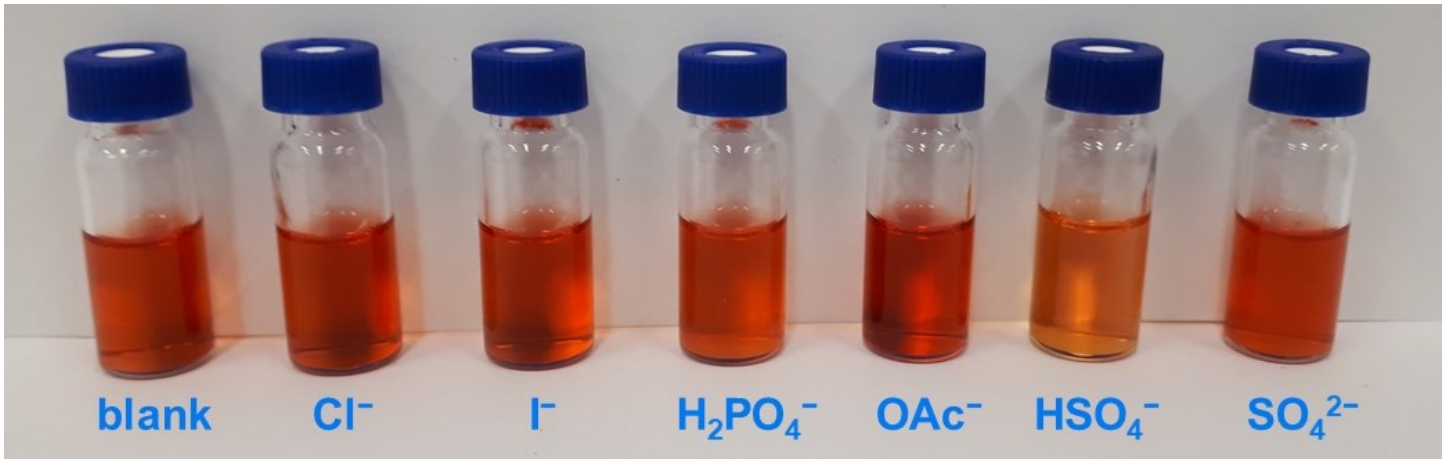

Figure S28. Photographs of 1.0 mM solutions of **3^{-H}·PF_6** with one equivalent of various anions as their TBA salts in 1:1 MeCN:MeOH.

Quantitative anion binding studies

General protocol

All anion binding titration experiments were conducted at 298 K. Initial sample volumes were 0.50 mL and concentrations were 2.0 mM of host. Solutions (100 mM) of anions as tetrabutylammonium salts were added in aliquots, the samples thoroughly shaken and spectra recorded at 0, 0.2, 0.4, 0.6, 0.8, 1.0, 1.2, 1.4, 1.6, 1.8, 2.0, 2.5, 3.0, 4.0, 5.0, 7.0 and 10 equivalents of anion. Data were fitted to 1:1 binding isotherms using the *Bindfit* program;[4] web-links to these isotherms are provided.

Anion binding data, NMR spectra and isotherms

The following graphs show the data and fitted isotherms used to determine association constants as well as stack plots showing the ^{1}H NMR spectra from which these data were obtained (Figures S29–48). These stack plots each contain spectra corresponding to the 17 datapoints described in the general protocol. Spectrum 1 (the bottom spectrum) corresponds to 0 equivalents of anion through to spectrum 17 (the top spectrum) corresponding to 10 equivalents of anion.

In titrations conducted in CD_3CN:CD_3OD or CD_3CN:D_2O, the receptors' O–H proton resonance disappears due to H/D exchange. In titrations conducted in CD_3CN, this proton also typically disappears: in the case of **2**$^+$, a very broad and weak resonance was visible and followed the same movement trend as the C–H protons. In the case of **1**$^+$, this peak could not be resolved.

1*⁺ *in CD_3CN

Cl^-	$K_a > 10^4\ M^{-1}$	http://app.supramolecular.org/bindfit/view/8cf7994d-6218-4e41-b6be-051aeba83763
SO_4^{2-}	*precipitation observed*	

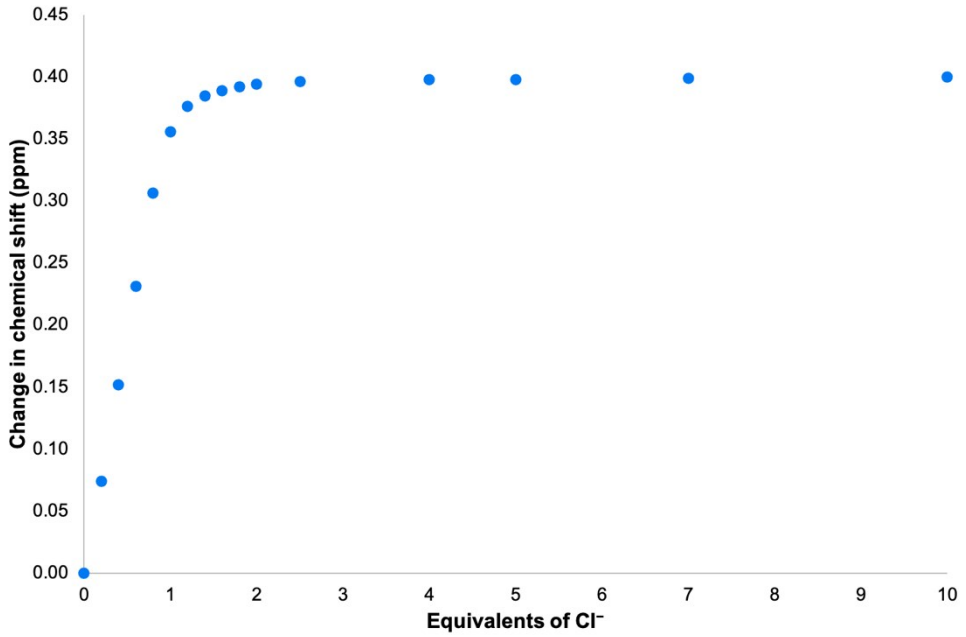

Figure S29. Movement of peak at 8.17 ppm upon addition of TBA·Cl (CD_3CN, 298 K).

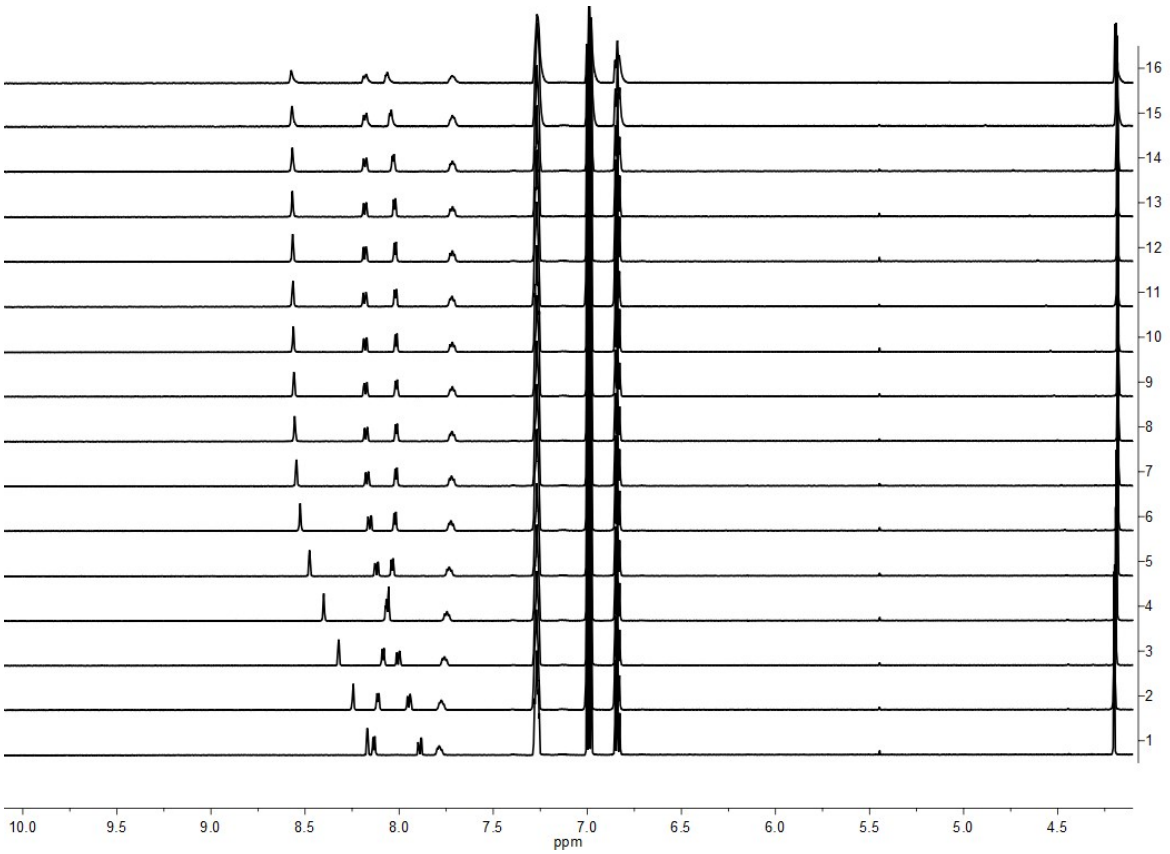

Figure S30. Truncated ^{1}H NMR spectra of **1·BPh_4** upon addition of increasing equivalents of TBA·Cl (CD_3CN, 298 K, 600 MHz). Note: a spectrum was accidentally not recorded for 3.0 equivalents of anion, hence there are only 16 spectra rather than 17.

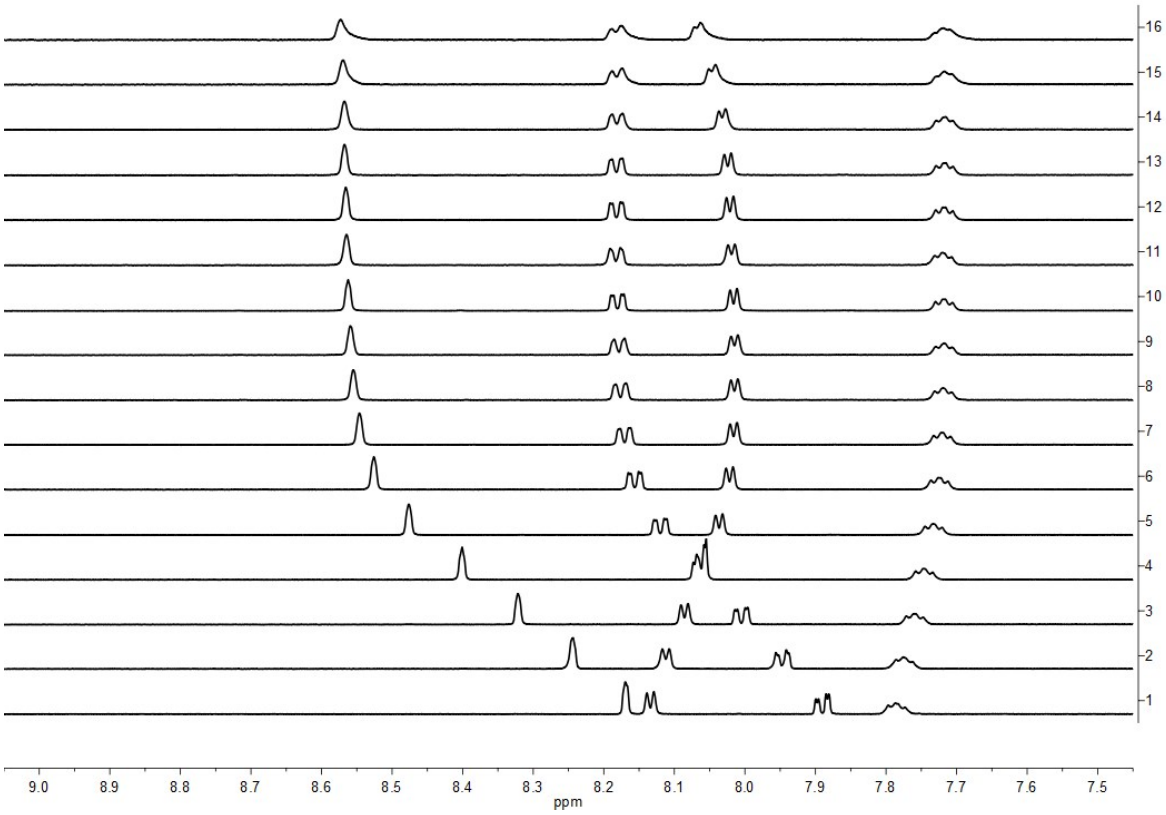

Figure S31. Truncated ^{1}H NMR spectra of **1·BPh$_4$** upon addition of increasing equivalents of TBA·Cl showing downfield region of the spectrum (CD_3CN, 298 K, 600 MHz). Note: a spectrum was accidentally not recorded for 3.0 equivalents of anion, hence there are only 16 spectra rather than 17.

2$^+$ in CD_3CN

Cl$^-$ $K_a > 10^4$ M^{-1} http://app.supramolecular.org/bindfit/view/e2918623-2fe9-4adc-a92a-c2b046056099
SO$_4^{2-}$ *precipitation observed*

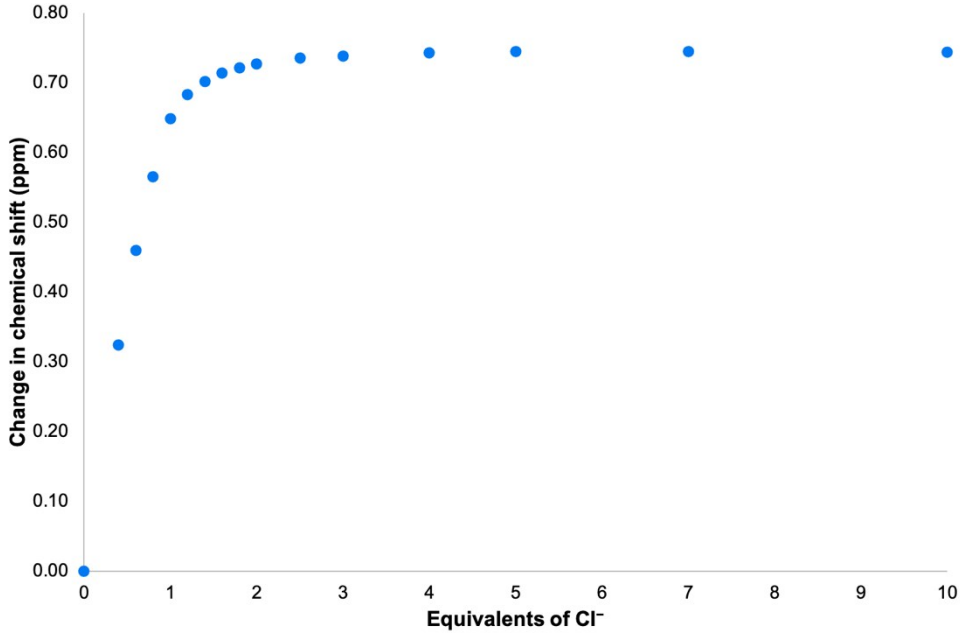

Figure S32. Movement of peak at 7.58 ppm upon addition of TBA·Cl (CD_3CN, 298 K).

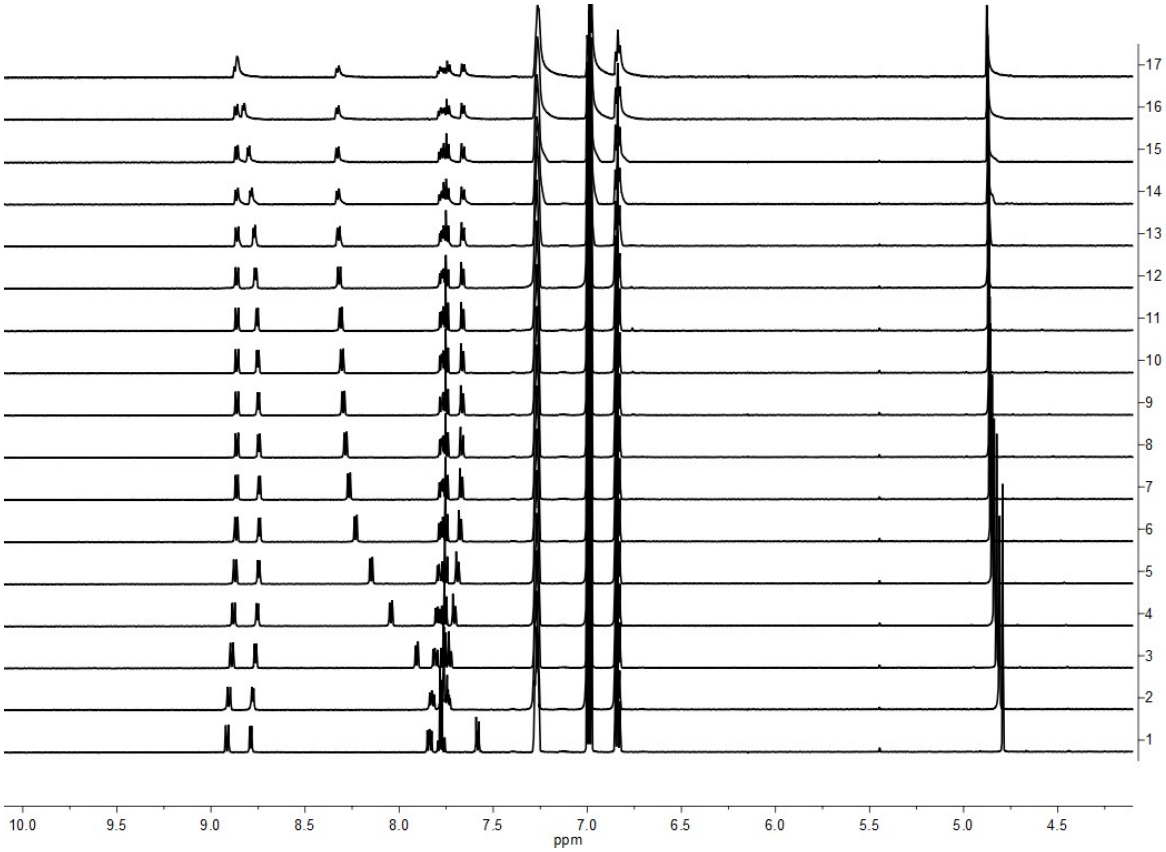

Figure S33. Truncated ^{1}H NMR spectra of **2·BPh$_4$** upon addition of increasing equivalents of TBA·Cl (CD_3CN, 298 K, 600 MHz).

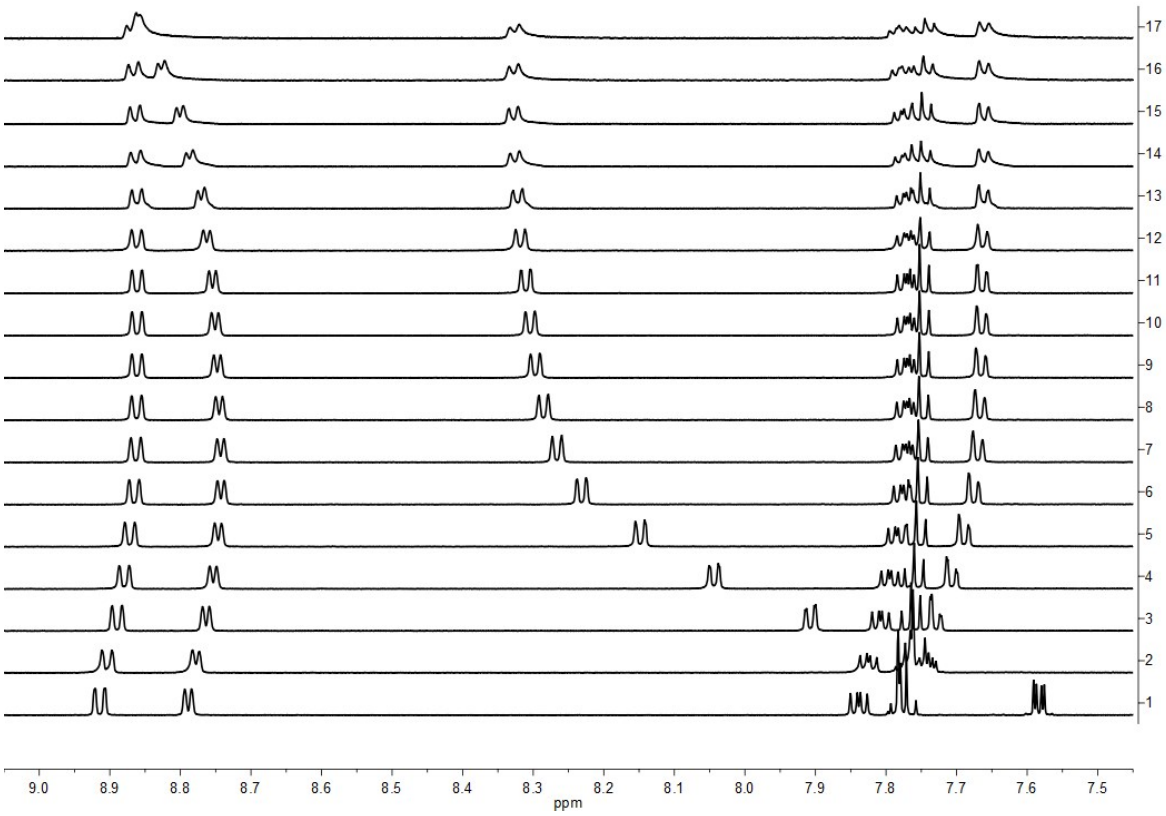

Figure S34. Truncated ^{1}H NMR spectra of **2·BPh$_4$** upon addition of increasing equivalents of TBA·Cl showing downfield region of the spectrum (CD_3CN, 298 K, 600 MHz).

1*⁺ *in 9:1 CD_3CN:D_2O

Cl^- K_a = 64.7 M^{-1} ± 3.9% http://app.supramolecular.org/bindfit/view/15110111-6f3e-4233-a173-fde1f4cce866
SO_4^{2-} K_a = 76.5 M^{-1} ± 11% http://app.supramolecular.org/bindfit/view/cd3f122b-94f2-454a-bb14-cd27849bdd64

Note: there is evidence of additional binding stoichiometries for binding of SO_4^{2-}, although attempts to fit 1:2 or 2:1 binding isotherms did not give sensible fits.

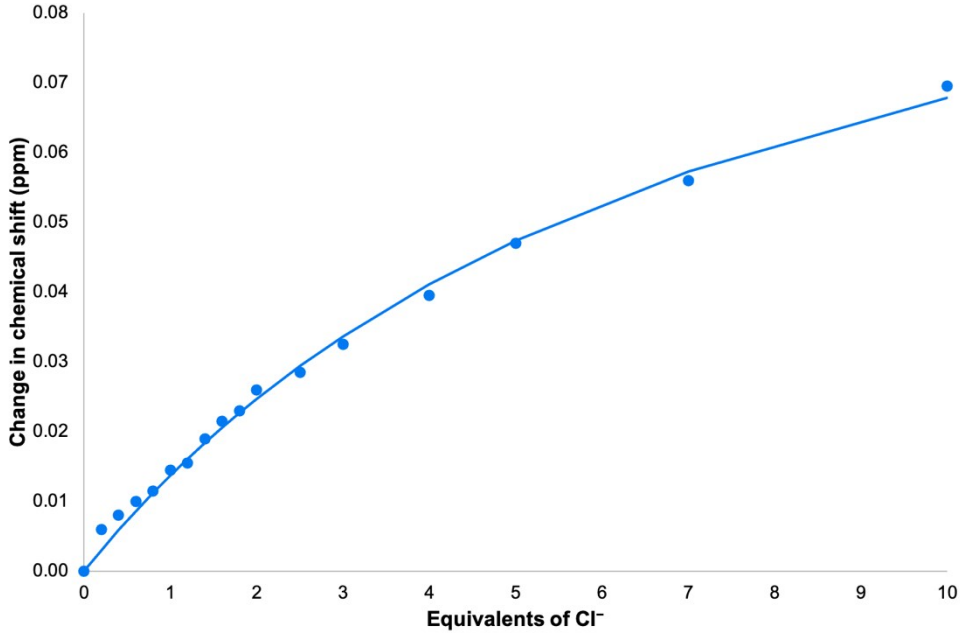

Figure S35. Movement of peak at 8.18 ppm upon addition of TBA·Cl (9:1 CD_3CN:D_2O, 298 K). Points represent observed data, line represents 1:1 isotherm calculated using *Bindfit*.[4]

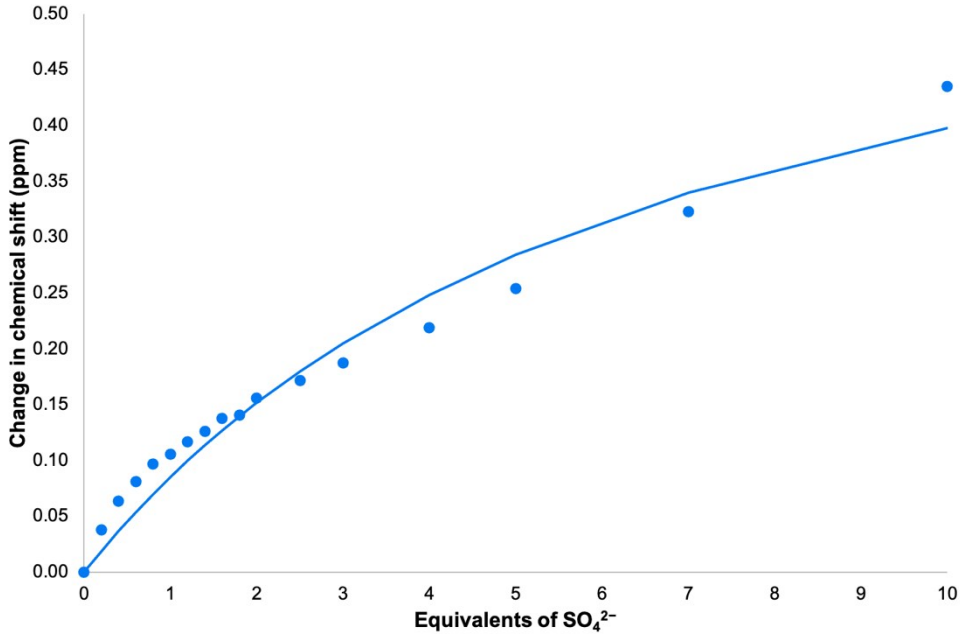

Figure S36. Movement of peak at 8.19 ppm upon addition of $TBA_2 \cdot SO_4$ (9:1 CD_3CN:D_2O, 298 K). Points represent observed data, line represents 1:1 isotherm calculated using *Bindfit*.[4] Note: there is clear evidence of stoichiometries other than 1:1 contibuting, although attempts to fit 1:2 or 2:1 isotherms were unsuccessful.

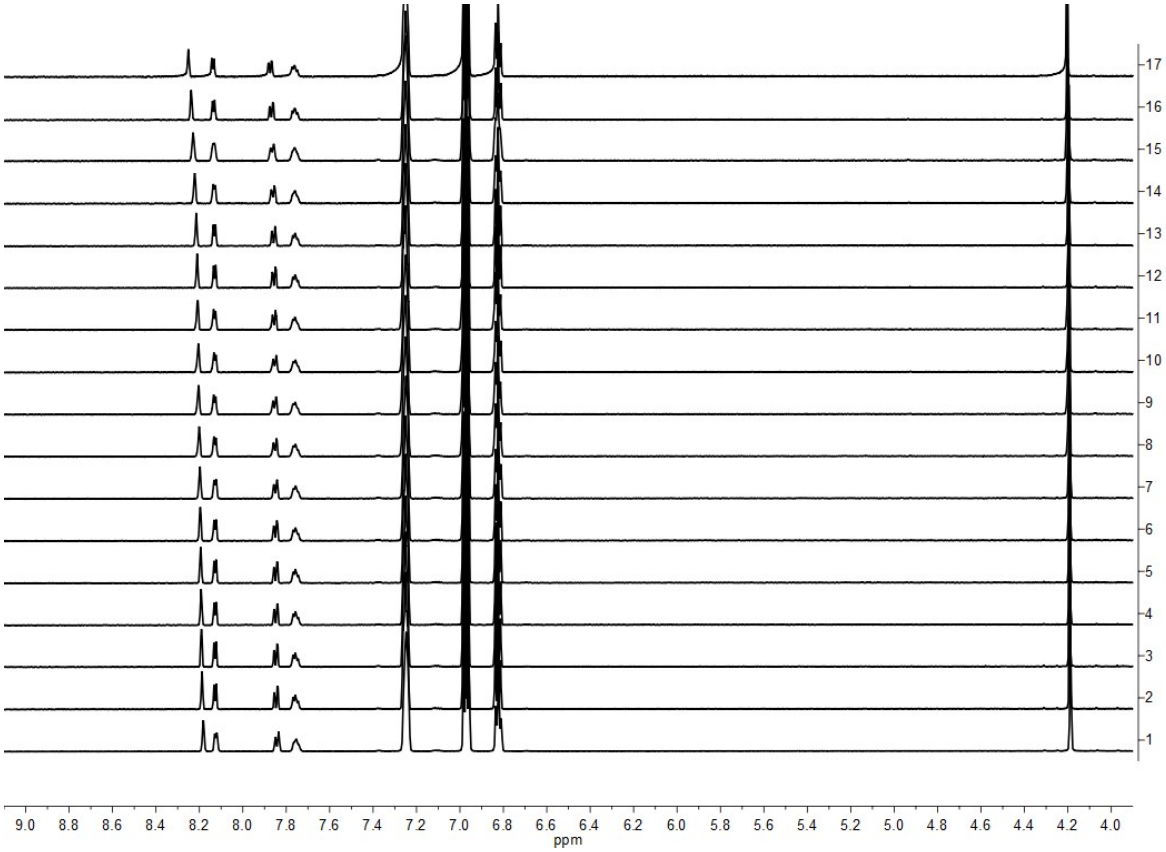

Figure S37. Truncated ^{1}H NMR spectra of **1·BPh$_4$** upon addition of increasing equivalents of TBA·Cl (9:1 CD_3CN:D_2O, 298 K, 600 MHz).

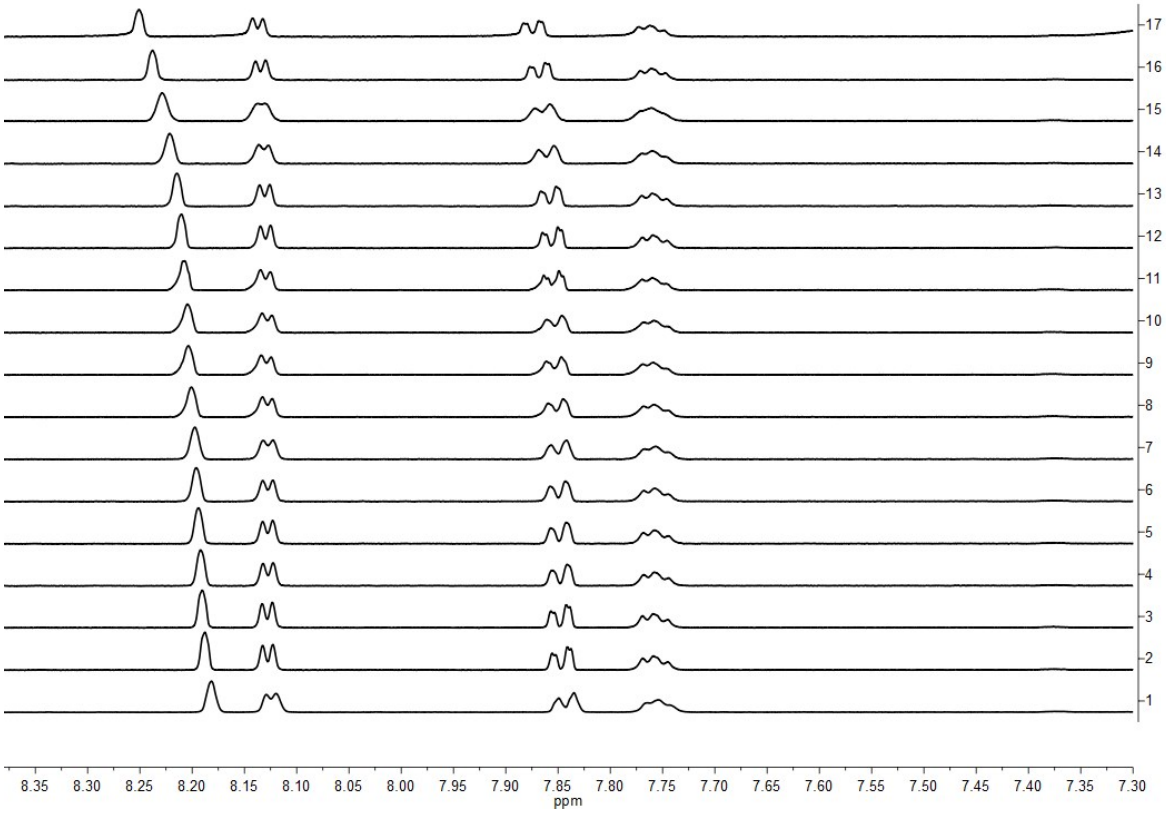

Figure S38. Truncated ^{1}H NMR spectra of **1·BPh$_4$** upon addition of increasing equivalents of TBA·Cl showing downfield region of the spectrum (9:1 CD_3CN:D_2O, 298 K, 600 MHz).

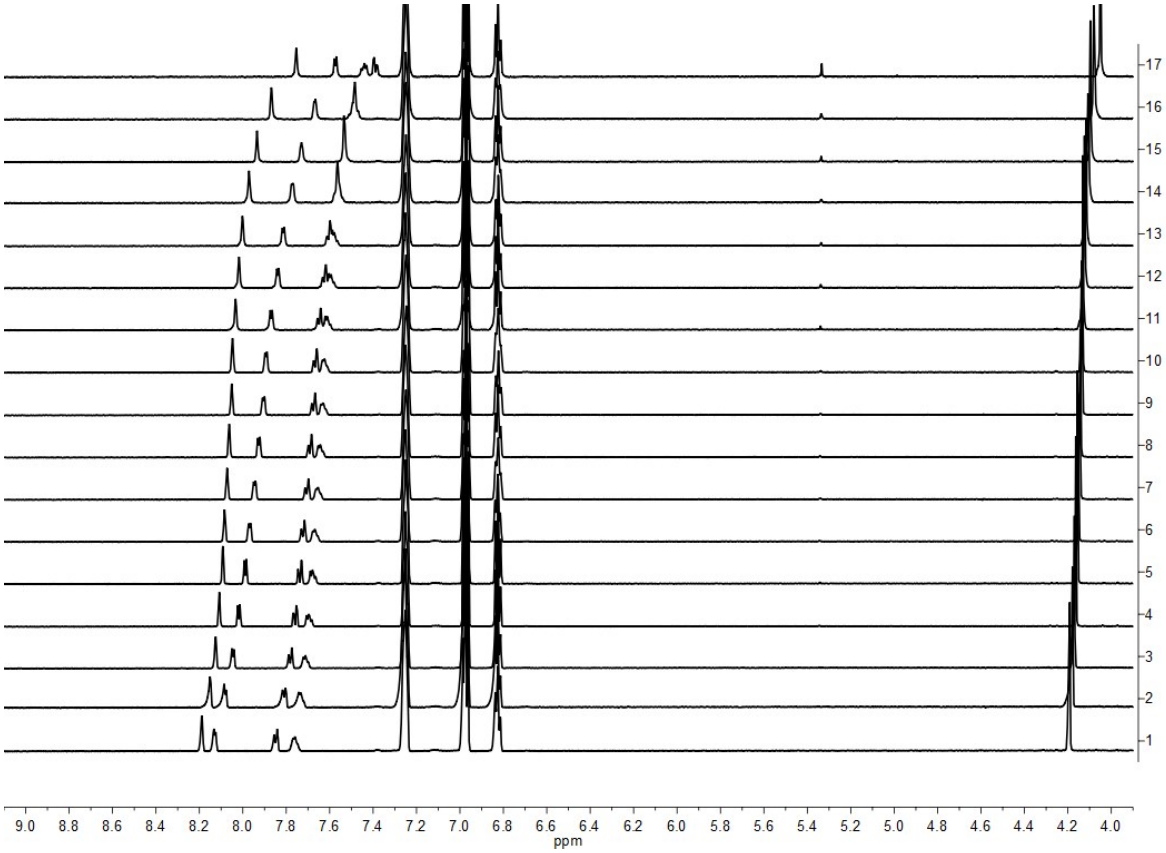

Figure S39. Truncated ^{1}H NMR spectra of **1·BPh$_4$** upon addition of increasing equivalents of $TBA_2{\cdot}SO_4$ (9:1 CD_3CN:D_2O, 298 K, 600 MHz).

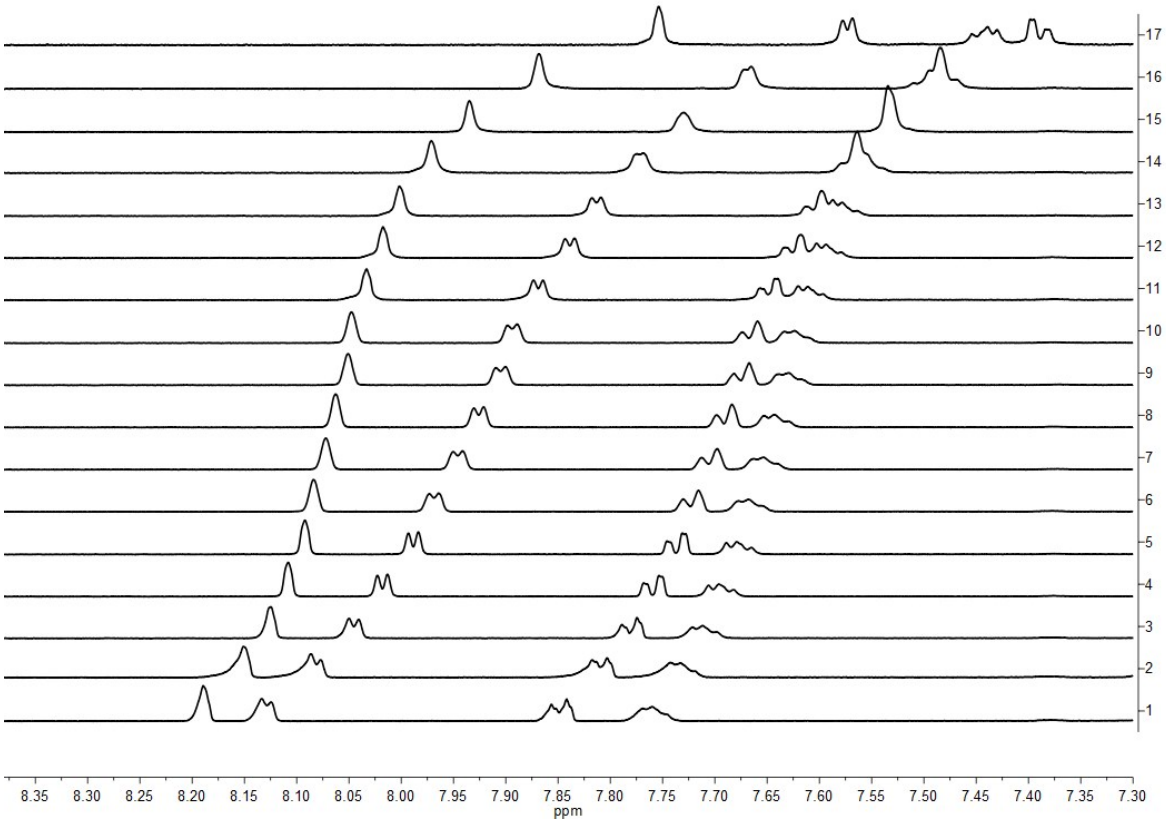

Figure S40. Truncated ^{1}H NMR spectra of **1·BPh$_4$** upon addition of increasing equivalents of $TBA_2{\cdot}SO_4$ showing downfield region of the spectrum (9:1 CD_3CN:D_2O, 298 K, 600 MHz).

2⁺ in 9:1 CD_3CN:D_2O

Cl^-	K_a = 12.6 M^{-1} ± 2.1%	http://app.supramolecular.org/bindfit/view/a963defe-a3ce-4c89-9917-ba8c238de345
SO_4^{2-}	K_a < 1 M^{-1}	http://app.supramolecular.org/bindfit/view/767b9586-12dc-402f-ac21-50f14c7c534d

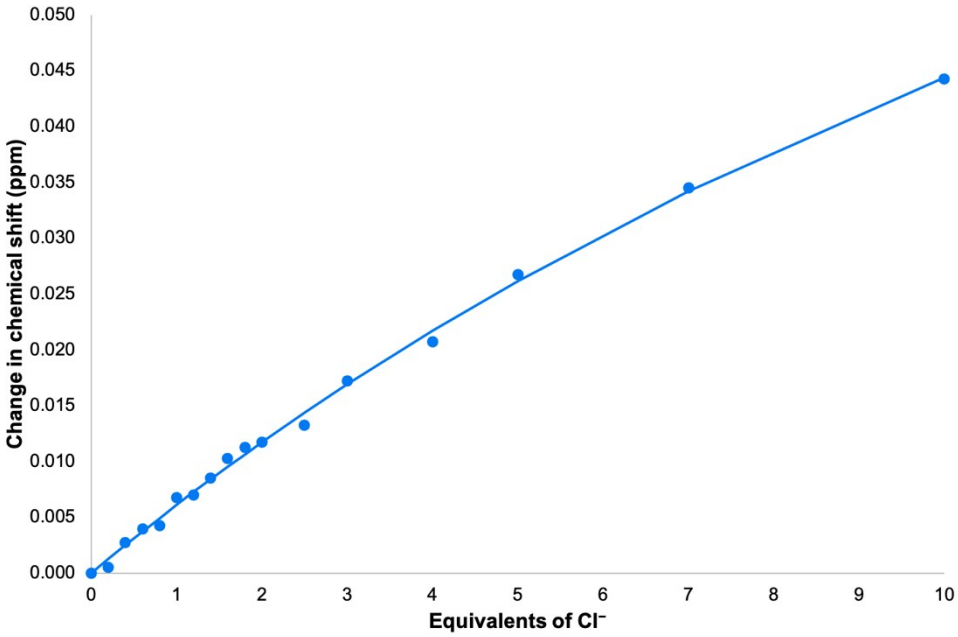

Figure S41. Movement of peak at 7.55 ppm upon addition of TBA·Cl (9:1 CD_3CN:D_2O, 298 K). Points represent observed data, line represents 1:1 isotherm calculated using *Bindfit*.[4]

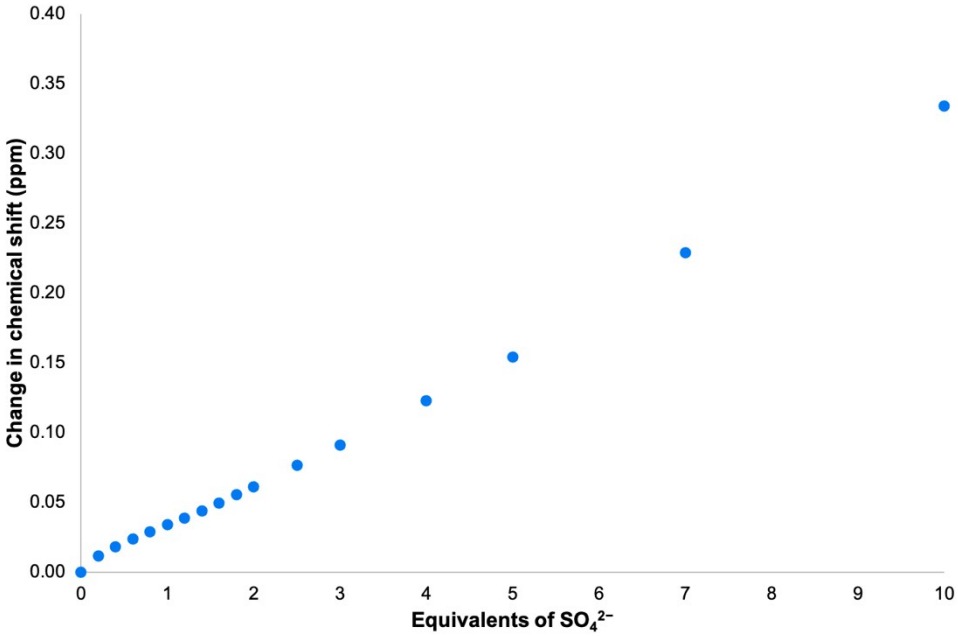

Figure S42. Movement of peak at 7.55 ppm upon addition of $TBA_2{\cdot}SO_4$ (9:1 CD_3CN:D_2O, 298 K).

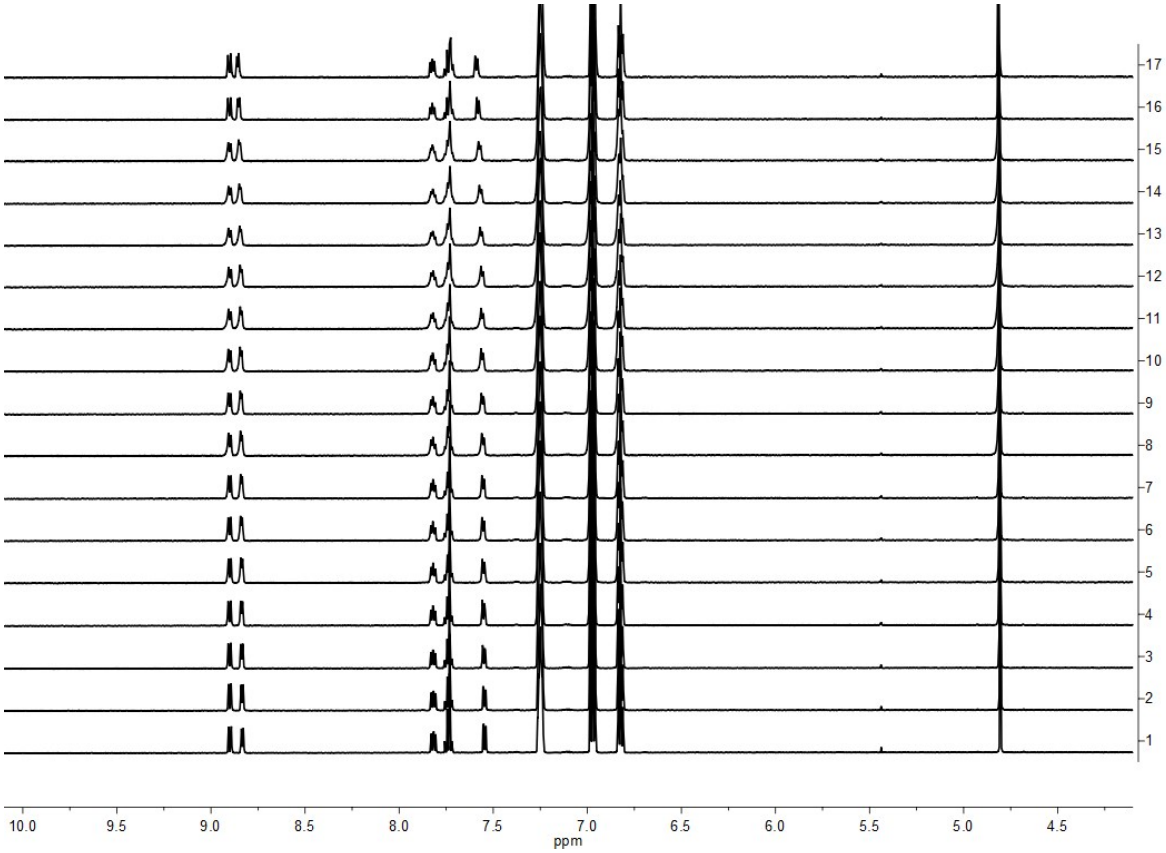

Figure S43. Truncated ^{1}H NMR spectra of **2·BPh$_4$** upon addition of increasing equivalents of TBA·Cl (9:1 CD_3CN:D_2O, 298 K, 600 MHz).

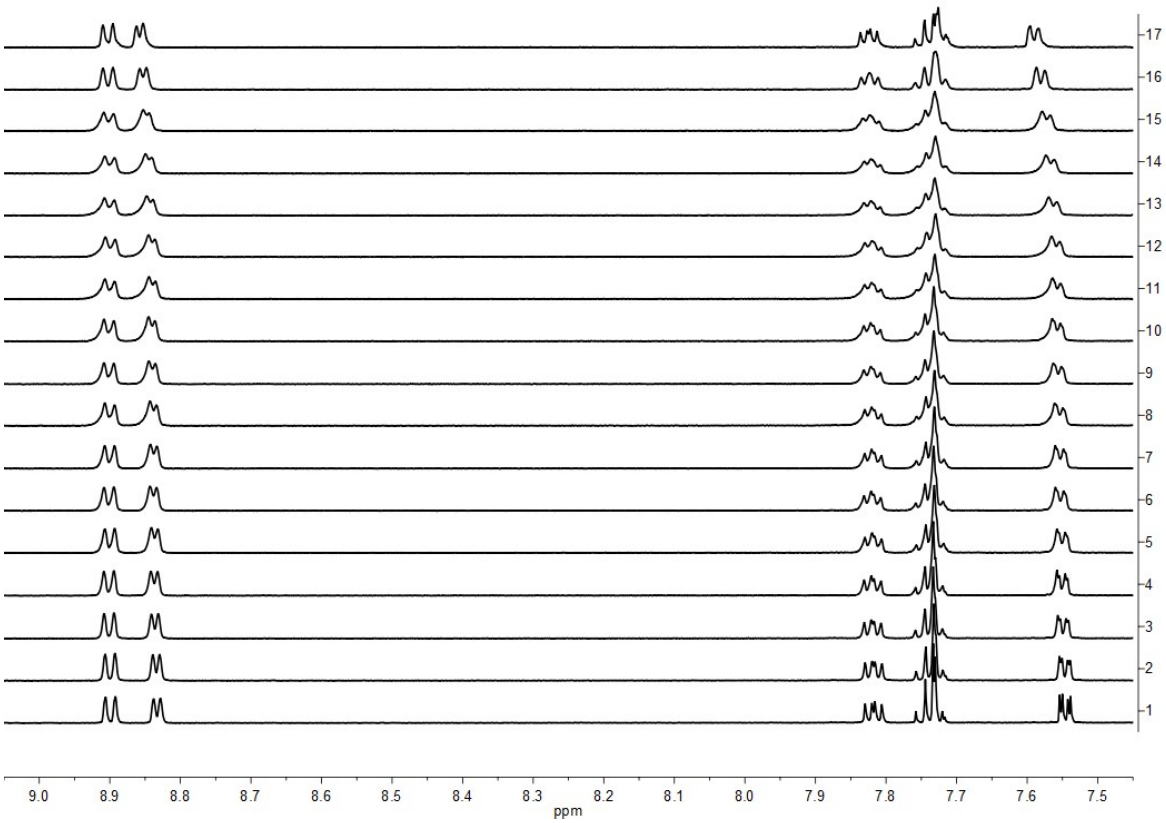

Figure S44. Truncated ^{1}H NMR spectra of **2·BPh$_4$** upon addition of increasing equivalents of TBA·Cl showing downfield region of the spectrum (9:1 CD_3CN:D_2O, 298 K, 600 MHz).

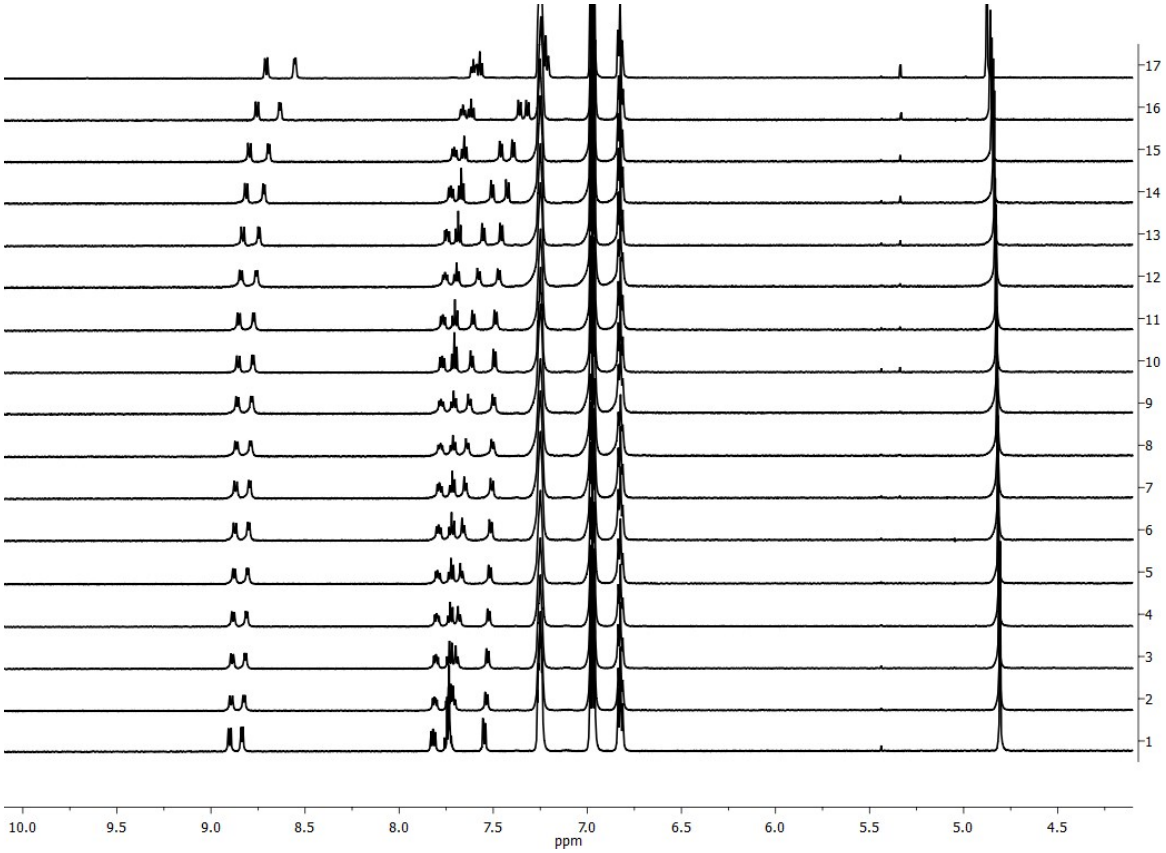

Figure S45. Truncated ^{1}H NMR spectra of **2·BPh$_4$** upon addition of increasing equivalents of $TBA_2{\cdot}SO_4$ (9:1 CD_3CN:D_2O, 298 K, 600 MHz).

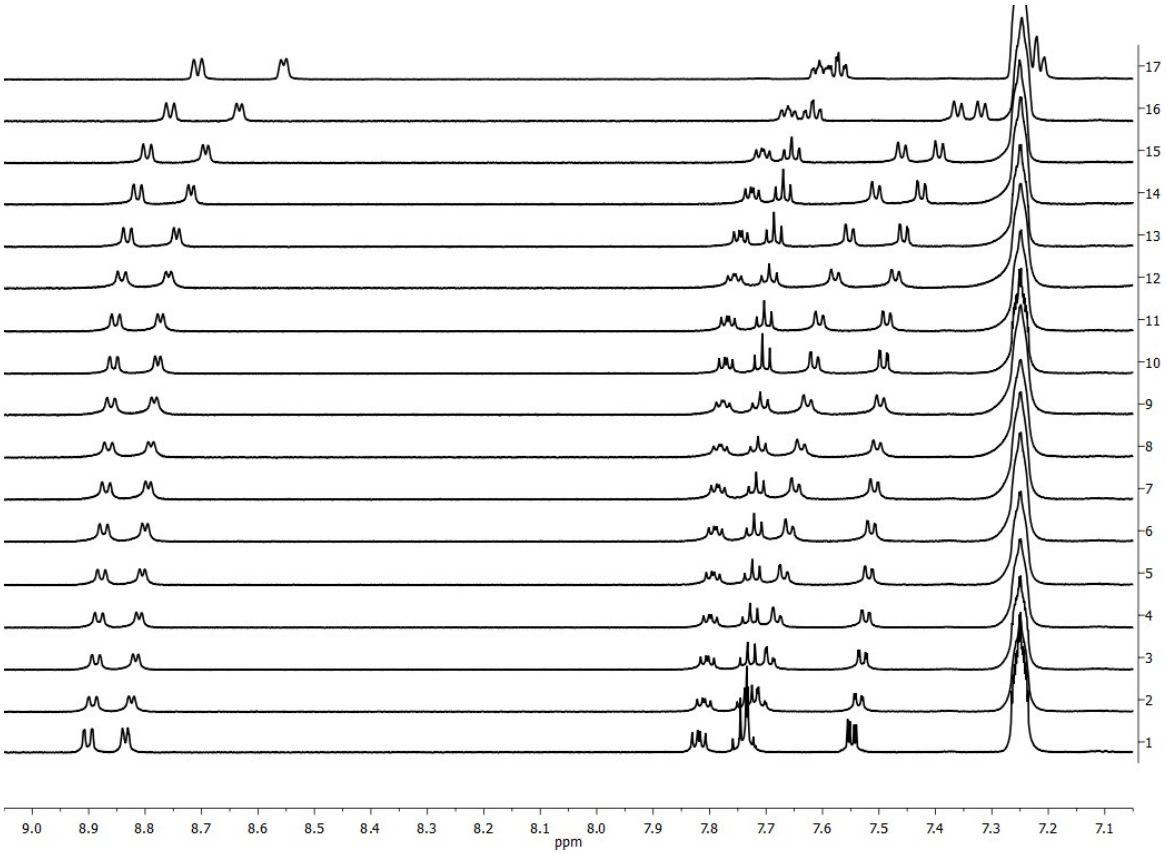

Figure S46. Truncated ^{1}H NMR spectra of **2·BPh$_4$** upon addition of increasing equivalents of $TBA_2{\cdot}SO_4$ showing downfield region of the spectrum (9:1 CD_3CN:D_2O, 298 K, 600 MHz).

3*$^{2+}$ *in 1:1 CD_3CN:CD_3OD

Cl^- K_a = 75.9 M^{-1} ± 2.2% http://app.supramolecular.org/bindfit/view/3ebcbbbd-3d4f-448f-8fd9-456ee33347a7
SO_4^{2-} *precipitation observed*

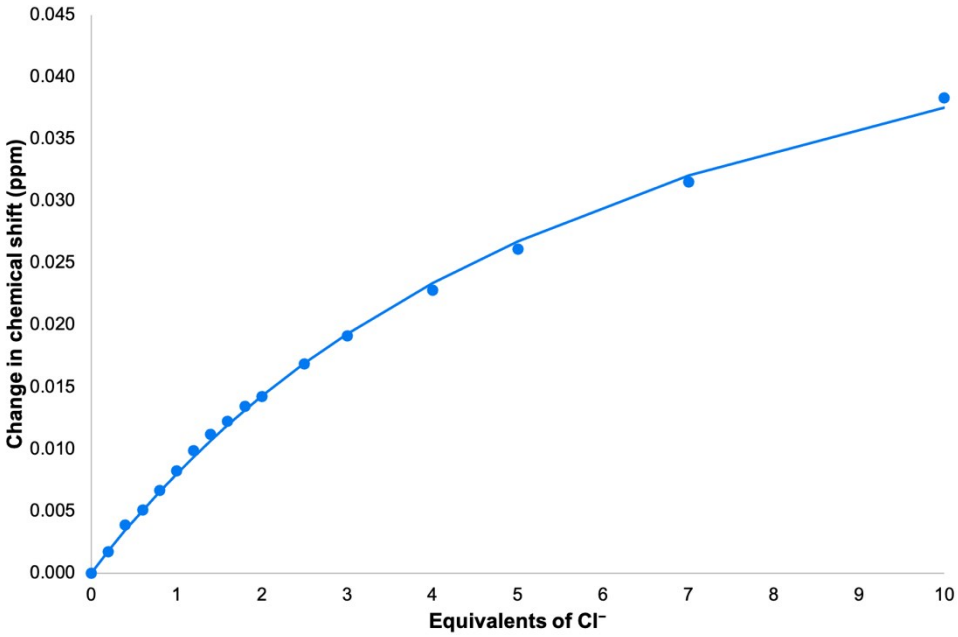

Figure S47. Movement of peak at 7.76 ppm upon addition of TBA·Cl (1:1 CD_3CN:CD_3OD, 298 K). Points represent observed data, line represents 1:1 isotherm calculated using *Bindfit*.[4]

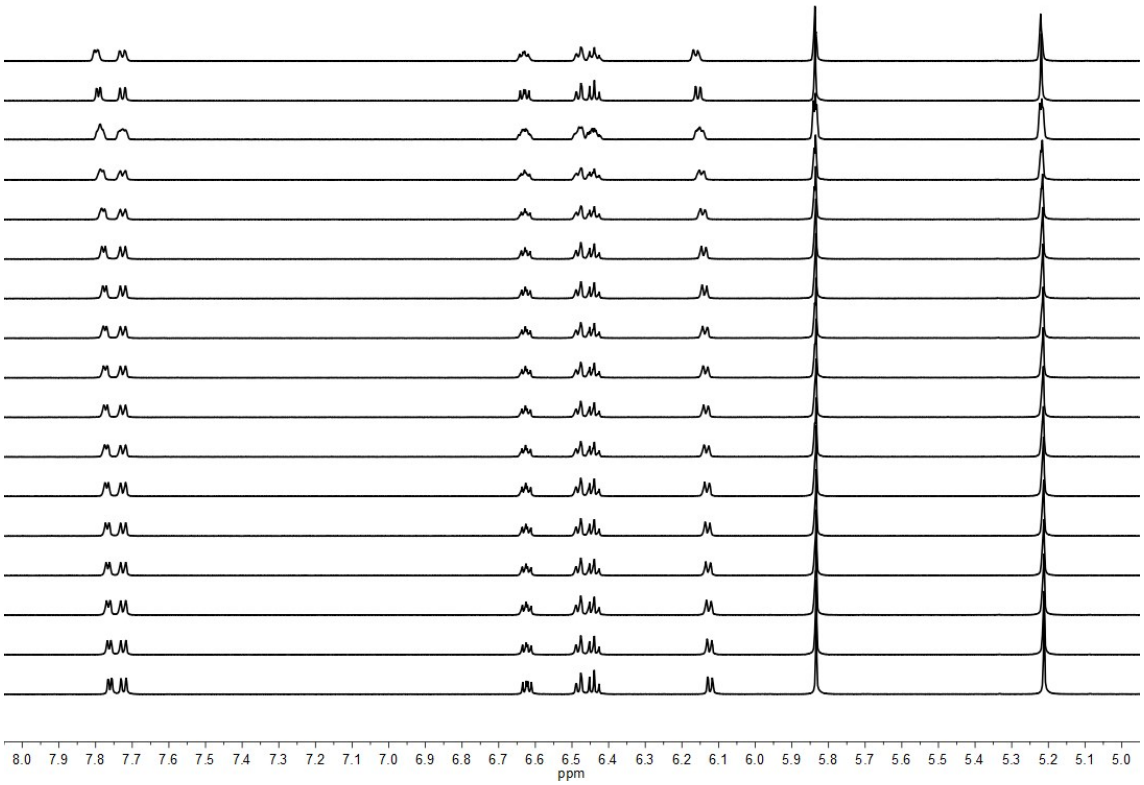

Figure S48. Truncated ^{1}H NMR spectra of **3·$(PF_6)_2$** upon addition of increasing equivalents of TBA·Cl (1:1 CD_3CN:CD_3OD, 298 K, 600 MHz).

Additional crystal structures

Structures of **1·BPh$_4$**, **2·PF$_6$·H$_2$O** and **3·(PF$_6$)$_2$·C$_3$H$_8$O** are shown in Figure S49. In the structure of **1·BPh$_4$**, the O–H group does not form any H-bond shorter than the sum of the van der Waals radii. The structure of **2·PF$_6$·H$_2$O** contains quite a short hydrogen bond between the receptor's O–H group and a water molecule (68% Σ_{vdW}[5]); this water molecule then forms a longer H-bond to the PF_6^- anion. In the structure of **3·(PF$_6$)$_2$·C$_3$H$_6$O**, the cation has an *anti* configuration with one O–H group forming a short H-bond to an acetone solvent molecule, while the other forms a longer H-bond to the PF_6^- anion (68% and 80% Σ_{vdW},[5] respectively). Generally, the structure is quite similar to **3·(PF$_6$)$_2$·(C$_2$H$_3$N)$_3$** (see main text) although in that structure both O–H groups hydrogen bond to solvent molecules.

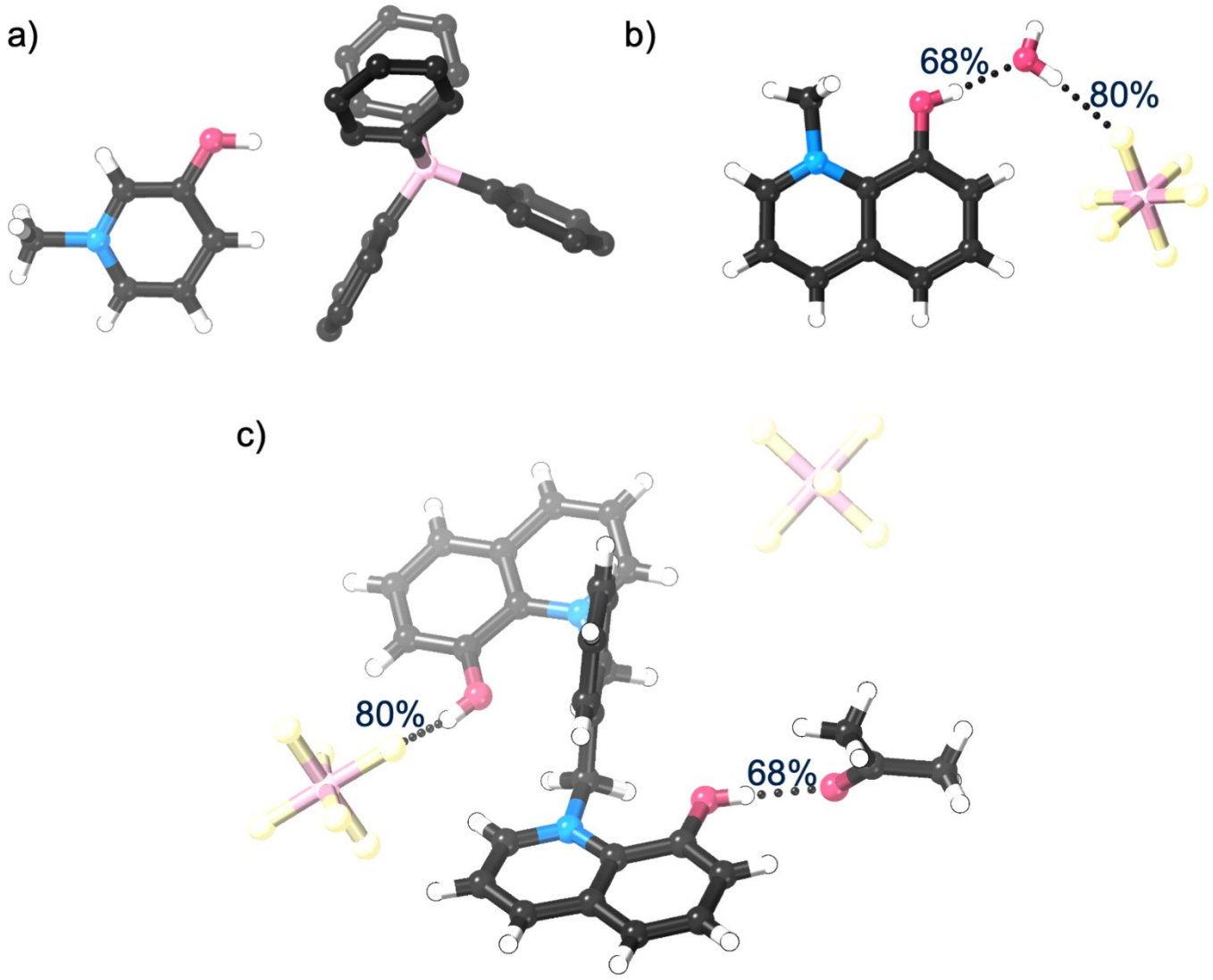

Figure S49. Structures of a) **1·BPh$_4$**, b) **2·PF$_6$·H$_2$O** and c) **3·(PF$_6$)$_2$·C$_3$H$_6$O.** H···acceptor distances for hydrogen bonds are given as Σ_{vdW}.[5]

The structure of $DBU^{H}{\cdot}PF_6$ is shown in Figure S50. Relatively long hydrogen bonds are formed between the amidinium N–H group and three fluorine atoms from a PF_6^- anion (90–92% Σ_{vdW}^5).

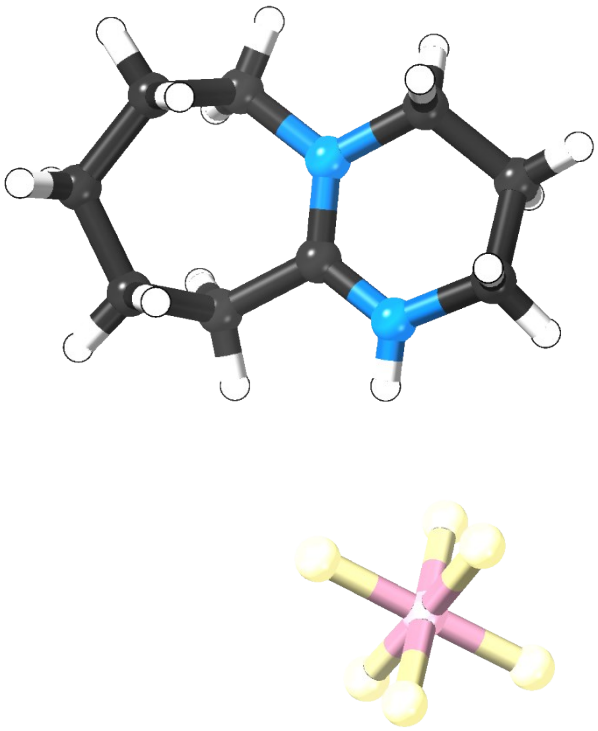

Figure S50. Structure of $DBU^{H}{\cdot}PF_6$.

X-ray crystallography

General remarks

Data for all structures except **3·SO$_4$** and DBU^H·PF$_6$ were collected using mirror-monochromated Cu Kα or Mo Kα radiation on an Agilent SuperNova or Agilent Xcalibur diffractometer at 150 K. Raw frame data (including data reduction, interframe scaling, unit cell refinement and absorption corrections) were processed using CrysAlisPro.[6] Data for DBU^H·PF$_6$ were collected using the MX1 beamline,[7] and data for **3·SO$_4$** were collected using the MX2 beamline[8] at the Australian Synchrotron at 100 K. Raw frame data (including data reduction, interframe scaling and unit cell refinement) were processed using XDS.[9]

All structures were solved with SUPERFLIP[10] and refined using full-matrix least-squares on F^2 within the CRYSTALS suite.[11] All non-hydrogen atoms were refined with anisotropic displacement parameters.

Unless otherwise stated, C–H hydrogen atoms were visible in the Fourier difference map, and were initially refined with restraints on bond lengths and angles, after which the positions were used as the basis for a riding model.[12] O–H hydrogen atoms were visible in the Fourier difference map and their positions were refined with restraints on bond lengths and angles.[12] Unless otherwise stated it was not necessary to add any crystallographic restraints to these refinements apart from the restraints on O–H hydrogen atom positions. Comments on individual structures are provided below.

Details and thermal ellipsoid plots

Thermal ellipsoid plots of the asymmetric units of crystal structures reported in this paper are shown in Figures S51–S64. In all cases, ellipsoids are shown at 50% probability levels, and hydrogen atoms are omitted for clarity.

1·BPh$_4$: Crystals were grown by diffusion of diethyl ether vapour into an acetone solution of the compound. Crystals diffracted poorly, and despite long collection times and the use of Cu radiation, data were still weak at high angle. Despite the low quality of the data, refinement proceeded smoothly, although it was necessary to add restraints to thermal and vibrational and ellipsoid parameters. Due to the relatively low quality of the data, hydrogen atoms were inserted at geometric positions and ride on the attached atoms.

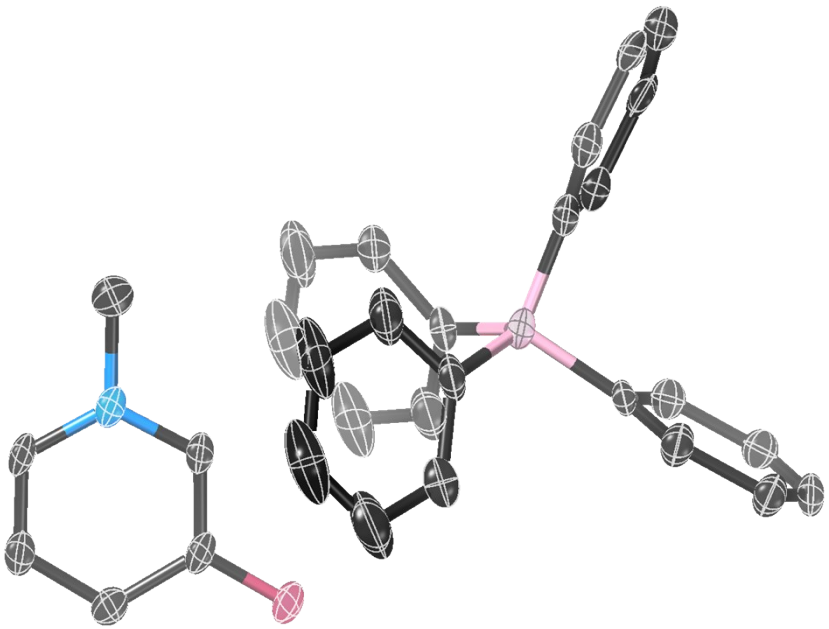

Figure S51. Thermal ellipsoid plot showing the asymmetric unit of **1·BPh$_4$**.

1·I: Crystals were grown by diffusion of diethyl ether vapour into an acetone solution of the compound. The compound has Z' = 5.

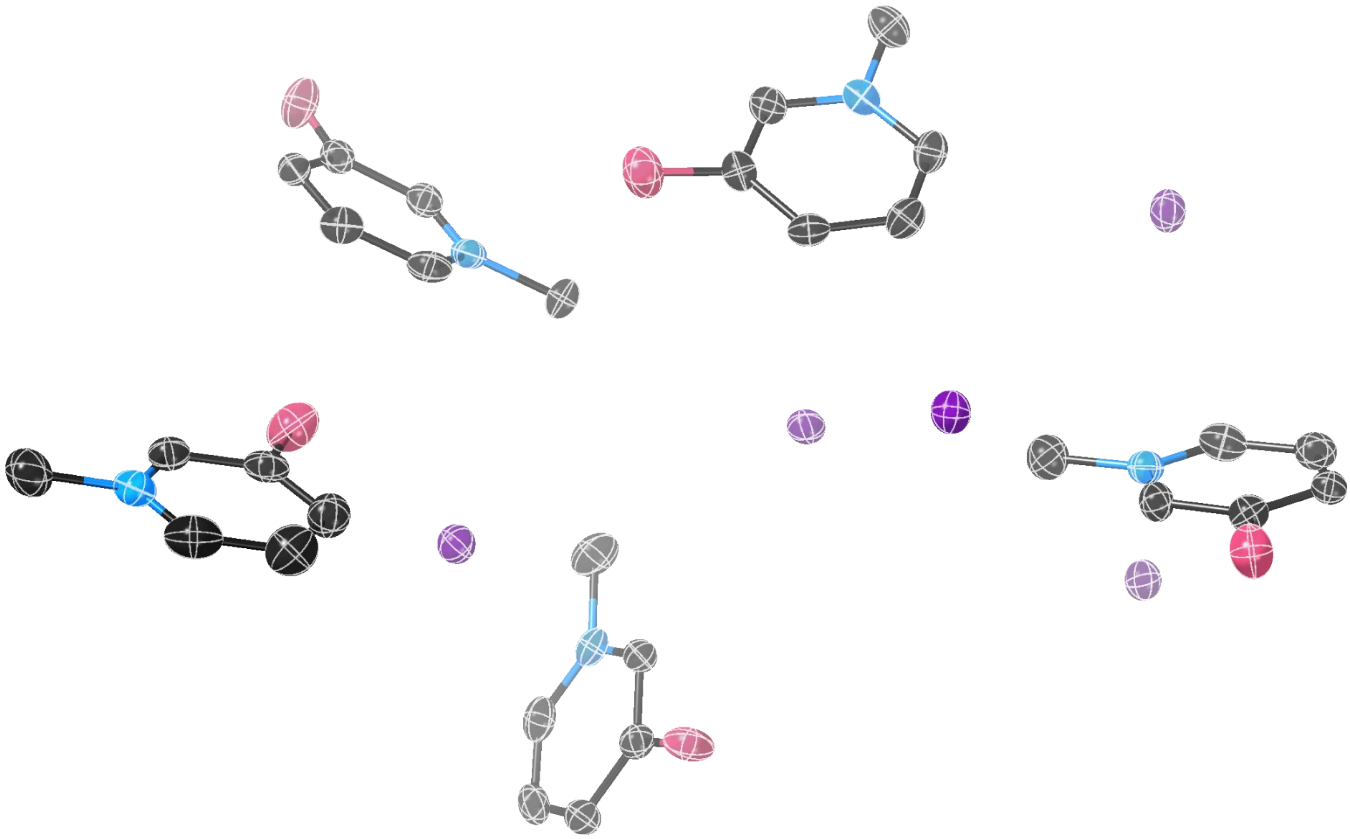

Figure S52. Thermal ellipsoid plot showing the asymmetric unit of **1·I.**

2·PF_6·H_2O: Crystals were grown by mixing concentrated hot aqueous solutions of **2·I** and NH_4PF_6 and allowing the resulting mixture to cool. Visually, this appeared to give a homogenous batch of crystals (which analysed by SCXRD as **2·PF_6·H_2O**), but analysis by ^{19}F NMR spectroscopy against a standard (2,2,2-trifluoroethanol) indicated that anion exchange was not complete. It seems likely that the bulk mixture is an approximately 1:1 mixture of **2·I** and **2·PF_6**.

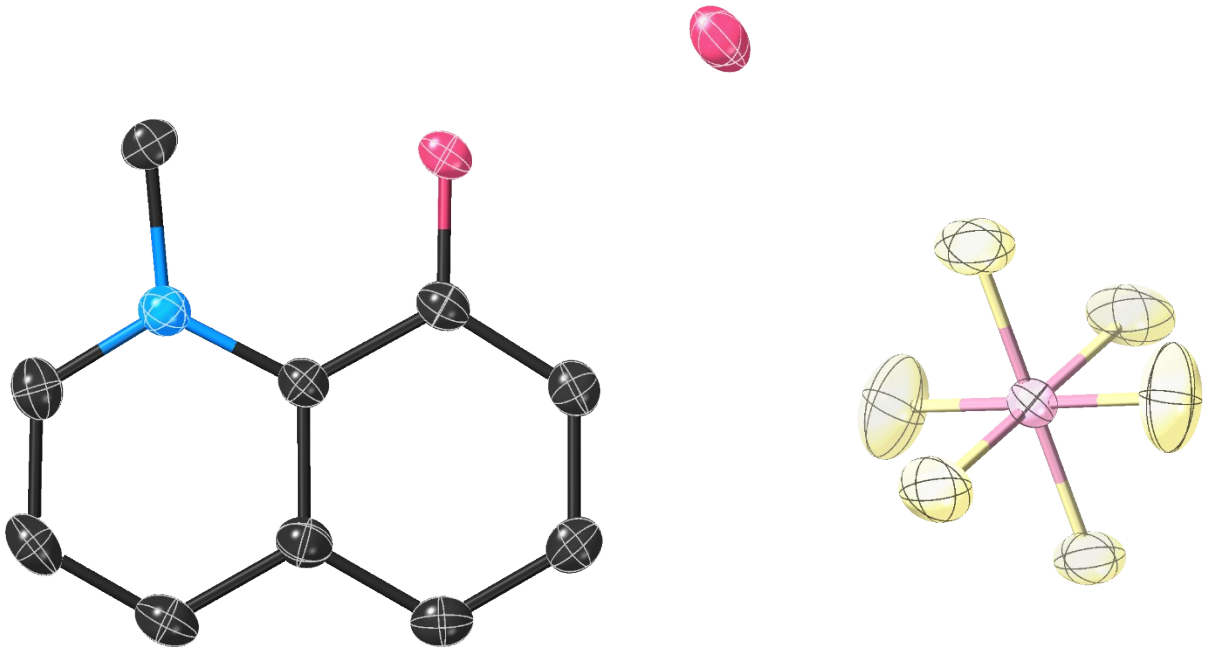

Figure S53. Thermal ellipsoid plot showing the asymmetric unit of **2·PF_6·H_2O**.

2·Cl: Crystals were grown by diffusion of diethyl ether vapour into a methanol solution of the compound.

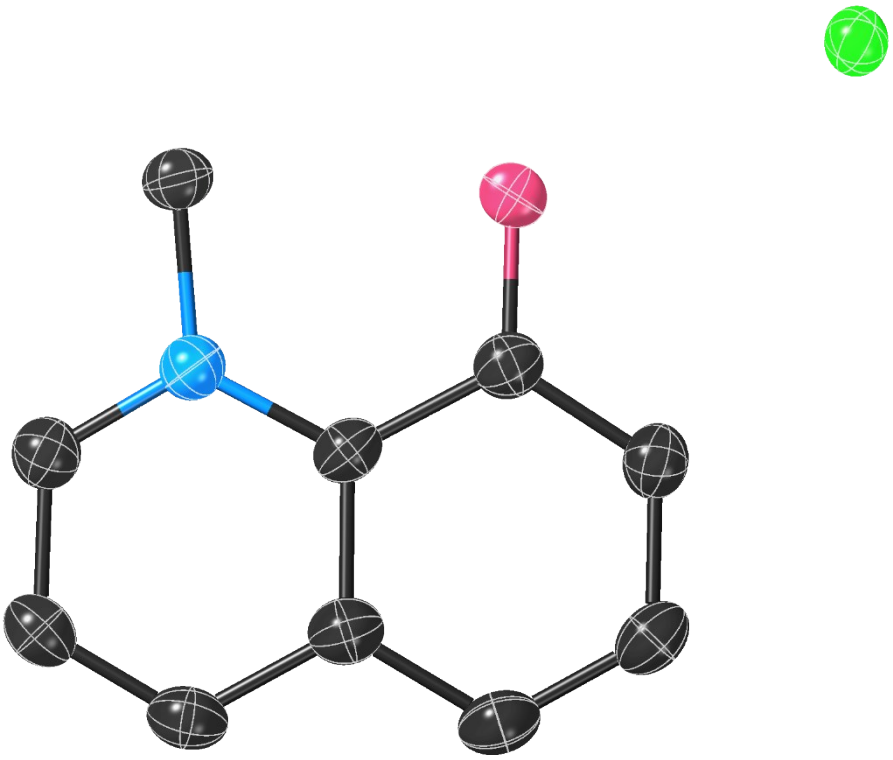

Figure S54. Thermal ellipsoid plot showing the asymmetric unit of **2·Cl**.

2_2·SO_4: Crystals were grown by diffusion of diethyl ether vapour into a methanol solution of the compound. The asymmetric unit contains one hydroxyquinolinium cation, and a sulfate anion located on a special position (such that overall there are two cations per anion).

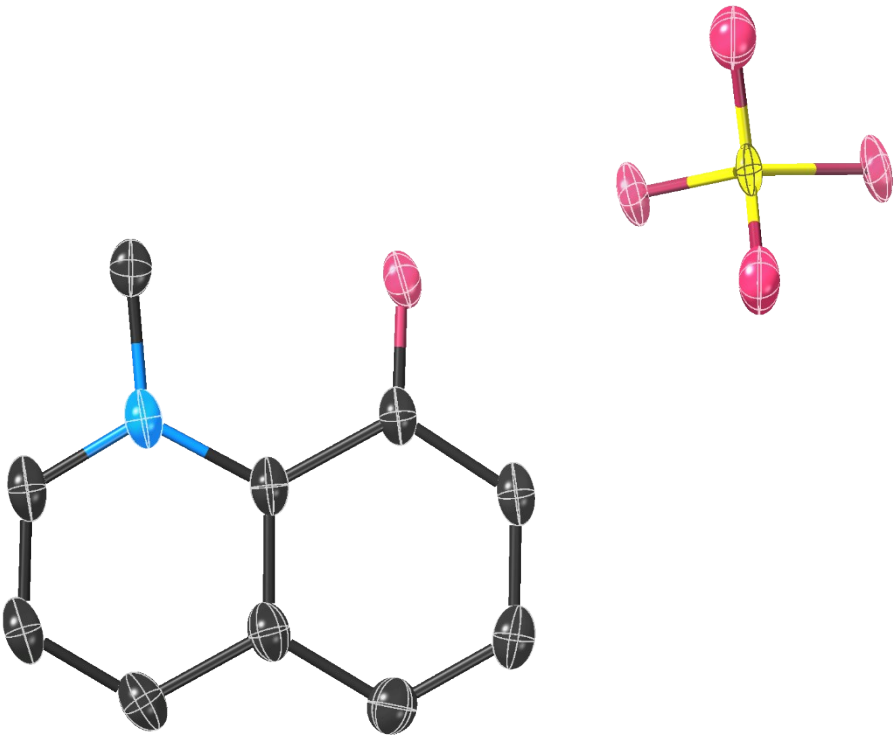

Figure S55. Thermal ellipsoid plot showing the asymmetric unit of **2_2·SO_4**.

$3\cdot(PF_6)_2\cdot C_3H_6O$: Crystals were grown by vapour diffusion of diethyl ether into an acetone solution of the compound.

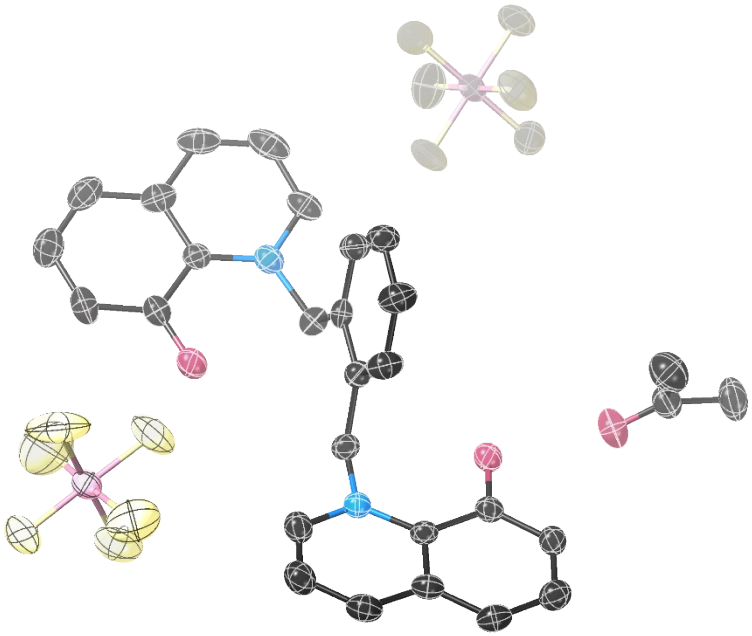

Figure S56. Thermal ellipsoid plot showing the asymmetric unit of **$3\cdot(PF_6)_2\cdot C_3H_6O$.**

$3\cdot(PF_6)_2\cdot(CH_3CN)_3$: Crystals were grown by vapour diffusion of diethyl ether into an acetonitrile solution of the compound. The asymmetric unit contains two $\mathbf{3}^{2+}$ cations, four PF_6^- anions, and six acetonitrile solvent molecules. One of the PF_6^- anions is disordered, and this was modelled by having two positions for the four equatorial fluorine atoms (occupancies: 0.6:0.4). It was necessary to apply restraints to the bond lengths and angles, as well as the thermal and vibrational and ellipsoid parameters of this disordered PF_6^- anion to achieve a sensible refinement.

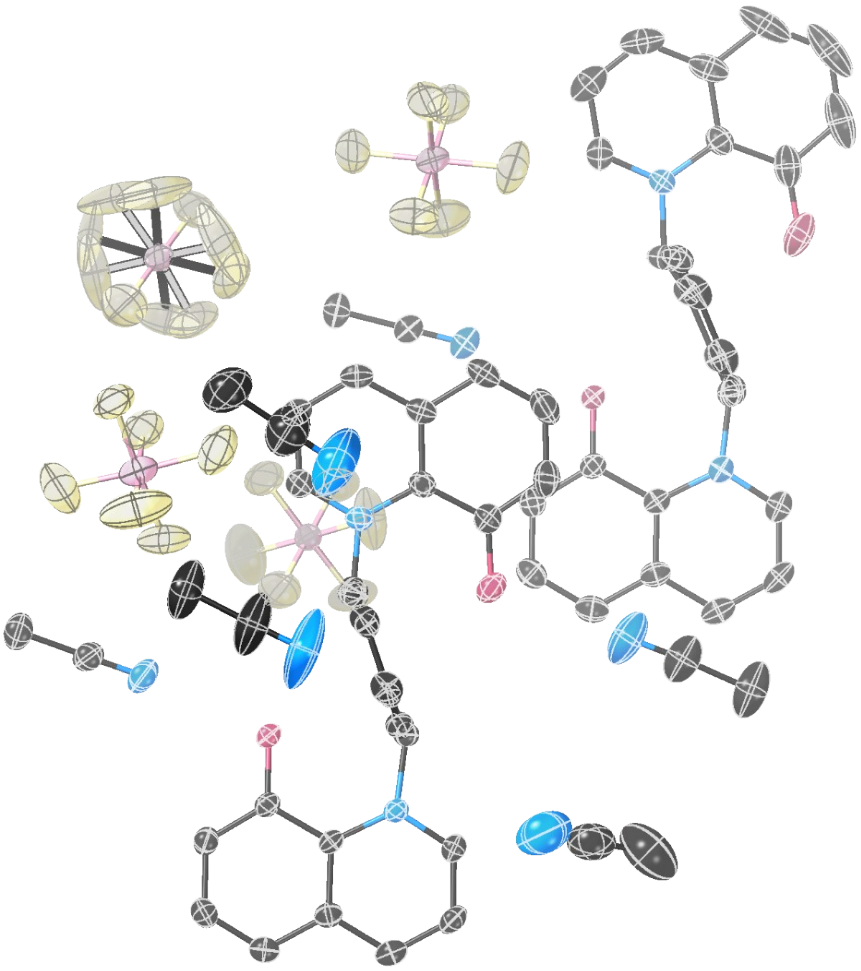

Figure S57. Thermal ellipsoid plot showing the asymmetric unit of **$3\cdot(PF_6)_2\cdot(CH_3CN)_6$**. Both positions of disordered PF_6^- anion shown.

3·Br_2: Crystals were grown by vapour diffusion of diethyl ether into a methanol solution of the compound. The structure has Z' = 0.5.

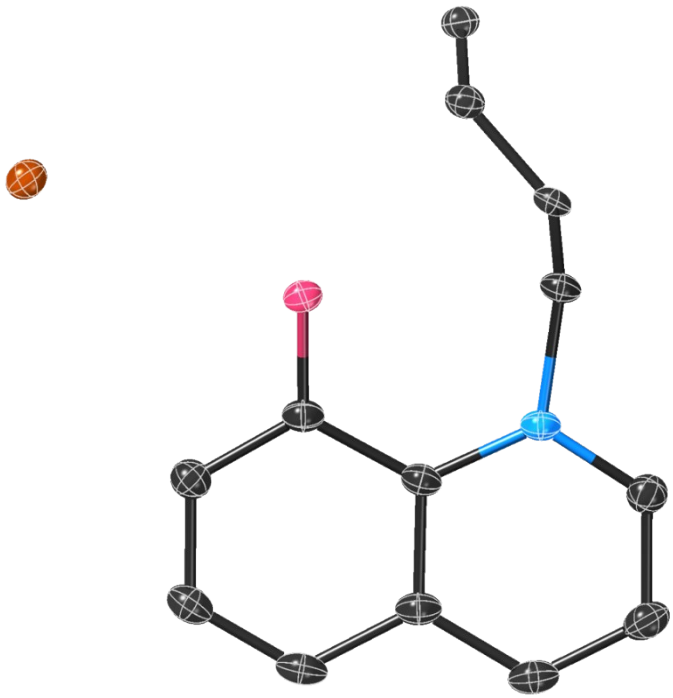

Figure S58 Thermal ellipsoid plot showing the asymmetric unit of **3·Br_2**.

3·Cl·PF_6·$(CH_3CN)_{0.5}$: Crystals were grown by vapour diffusion of diethyl ether into a solution containing **3·$(PF_6)_2$** and approximately one equivalent of tetrabutylammonium chloride in a mixture of acetonitrile and methanol. The structure contains one acetonitrile molecule located across a special position.

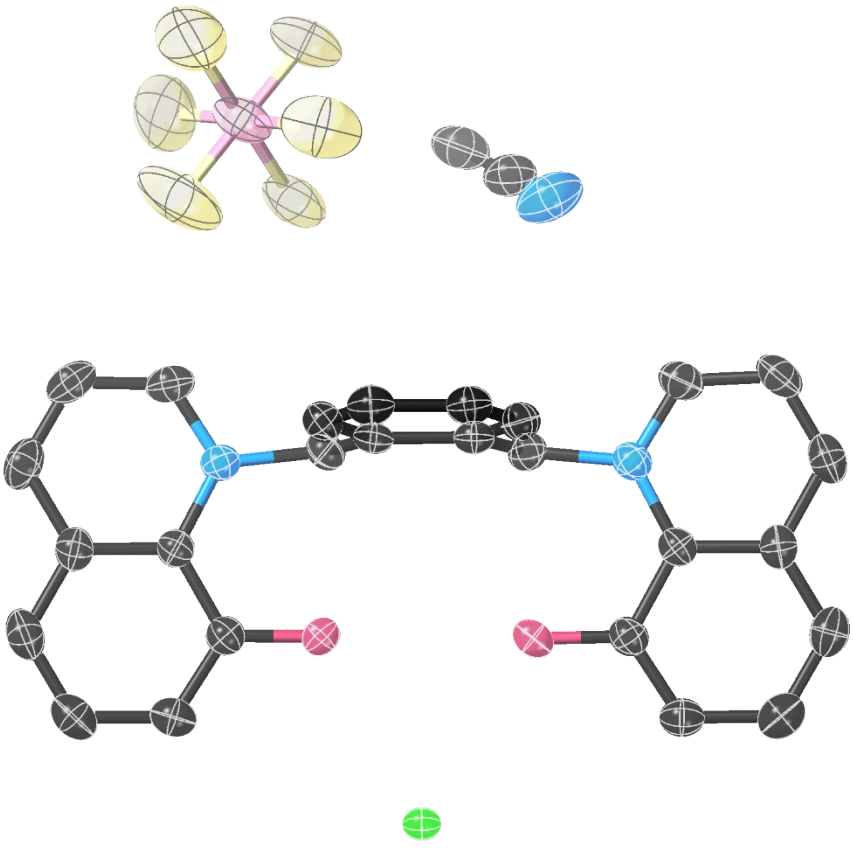

Figure S59. Thermal ellipsoid plot showing the asymmetric unit of **3·Cl·PF_6·$(CH_3CN)_{0.5}$**.

3·Br·PF_6·CH_3CN: Crystals were grown by vapour diffusion of diethyl ether into a solution containing **3·$(PF_6)_2$** and approximately one equivalent of tetrabutylammonium bromide in a mixture of acetonitrile and methanol. The PF_6^- anion exhibits positional disorder, which was modelled by having two positions for the four equatorial fluorine atoms (occupancies: 0.75:0.25).

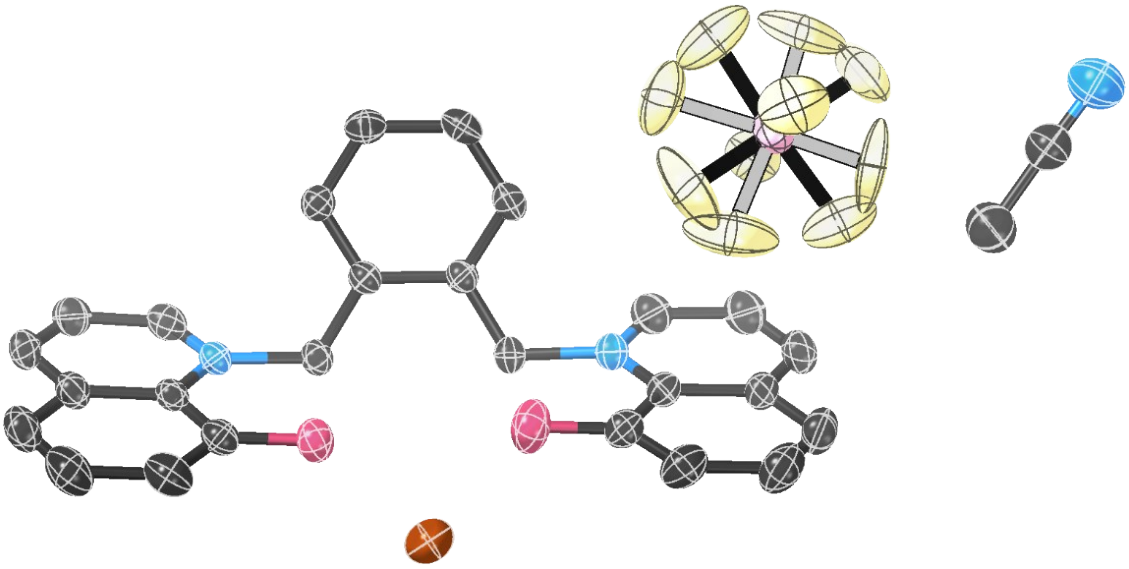

Figure S60. Thermal ellipsoid plot showing the asymmetric unit of **3·Br·PF_6·CH_3CN.** Both positions of disordered PF_6^- anion shown (occupancy 0.75:0.25).

3·SO_4·$(CH_3OH)_2$: Crystals were grown by adding one equivalent of TBA·HSO_4 to a 1.0 mM solution of **3^{-H}·PF_6** in 1:1 CH_3CN:CH_3OH. Crystals were very small and required the use of synchrotron radiation. Two methanol solvates are present in the asymmetric unit. O–H hydrogen atoms were not clearly visible in the difference map, so were initially inserted at idealised hydrogen bonding positions and then refined with restraints on O–H distances and C–O–H angles.

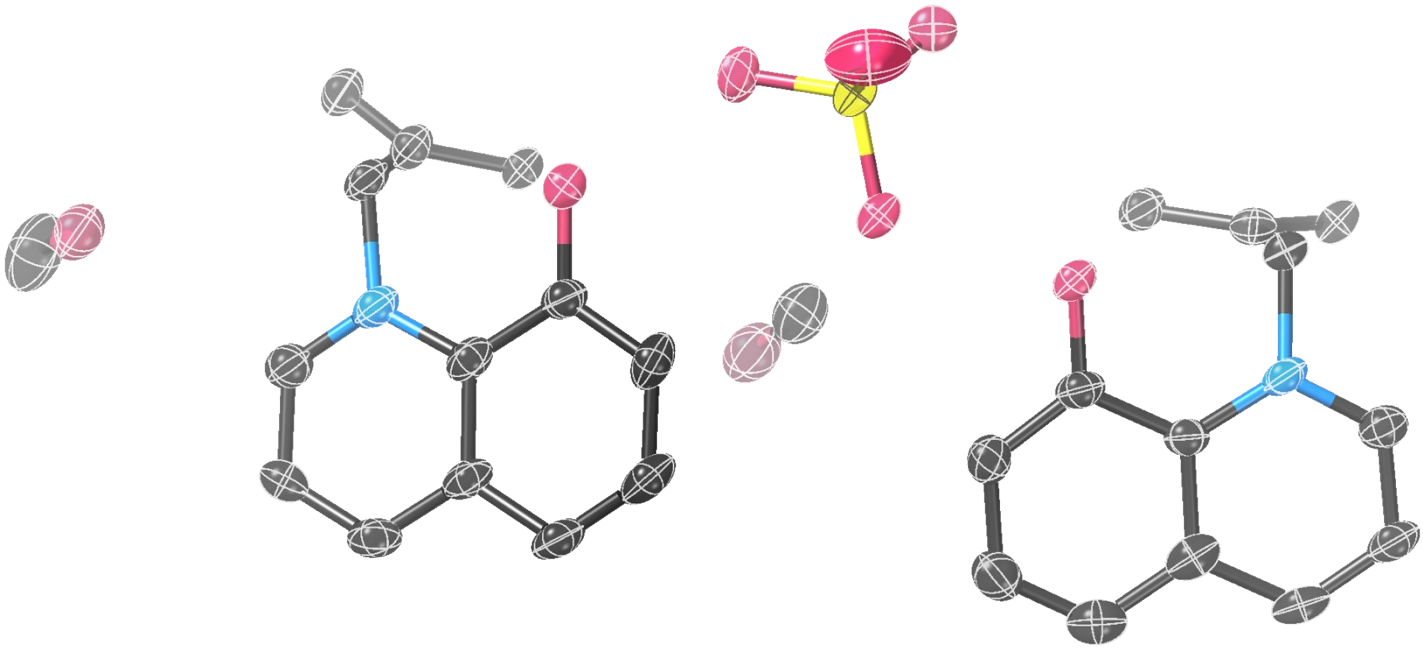

Figure S61. Thermal ellipsoid plot showing the asymmetric unit of **3·SO_4·$(CH_3OH)_2$**.

$3^{-H}\cdot PF_6$: Crystals were grown by vapour diffusion of diethyl ether into a solution containing **$3\cdot(PF_6)_2$** and approximately one equivalent of tetrabutylammonium iodide in a mixture of acetonitrile and methanol; this gave bright orange crystals of **$3^{-H}\cdot PF_6$** – it is unclear what has acted as base to deprotonate **3^{2+}**. Crystals having the same unit cell could be obtained by adding "NH_4PF_6" from an old bottle to **$3\cdot Br_2$** in methanol. As described in the main text, ^{19}F NMR spectroscopy revealed that the NH_4PF_6 was contaminated with significant amounts of F^-, which we believe acts as base to deprotonate **3^{2+}**. A region of diffuse electron density, believed to arise from disordered molecules, is located about a special position, and could not be refined sensibly so PLATON-SQUEEZE[13] was used to include this electron density in the refinement.

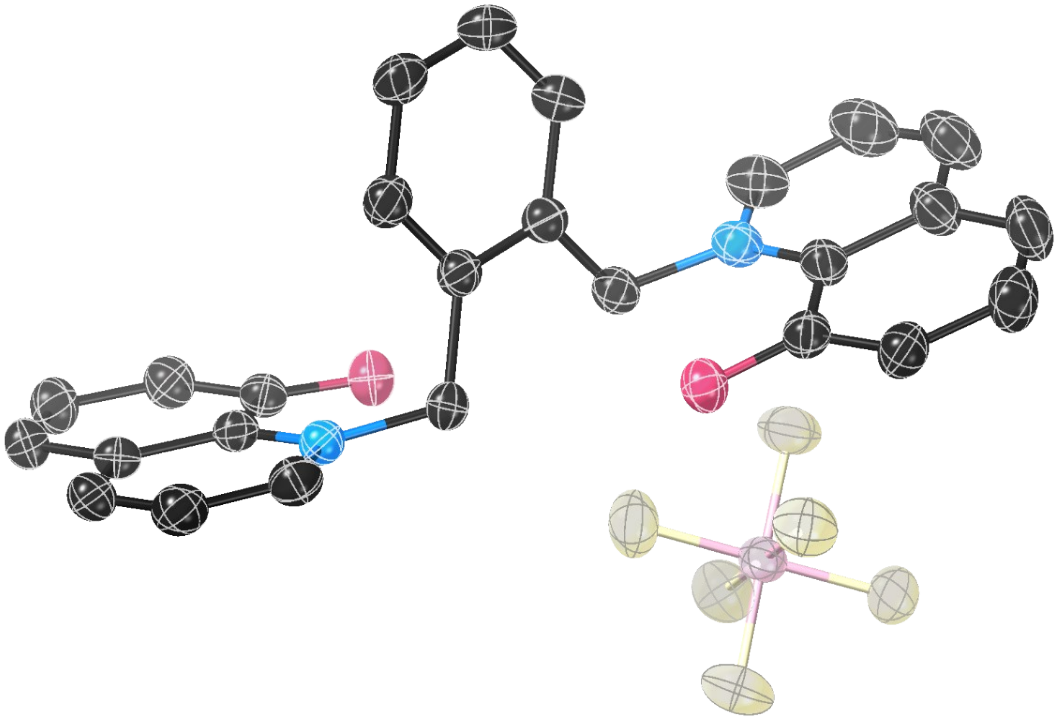

Figure S62. Thermal ellipsoid plot showing the asymmetric unit of **$3^{-H}\cdot PF_6$.** PLATON-SQUEEZE was used.[13]

$4\cdot Br\cdot CH_3CN$: A 1:2 molar ratio of dibromoxylene and 8-hydroxyquinoline were heated to reflux in acetonitrile for 48 hours and then cooled to room temperature. A yellow powder precipitated during the reaction. This was isolated by decanting, and the supernatant solution was left to stand. Over the course of a couple of hours, very large (*ca.* 3 mm in each direction) block-like crystals precipitated from the solution.

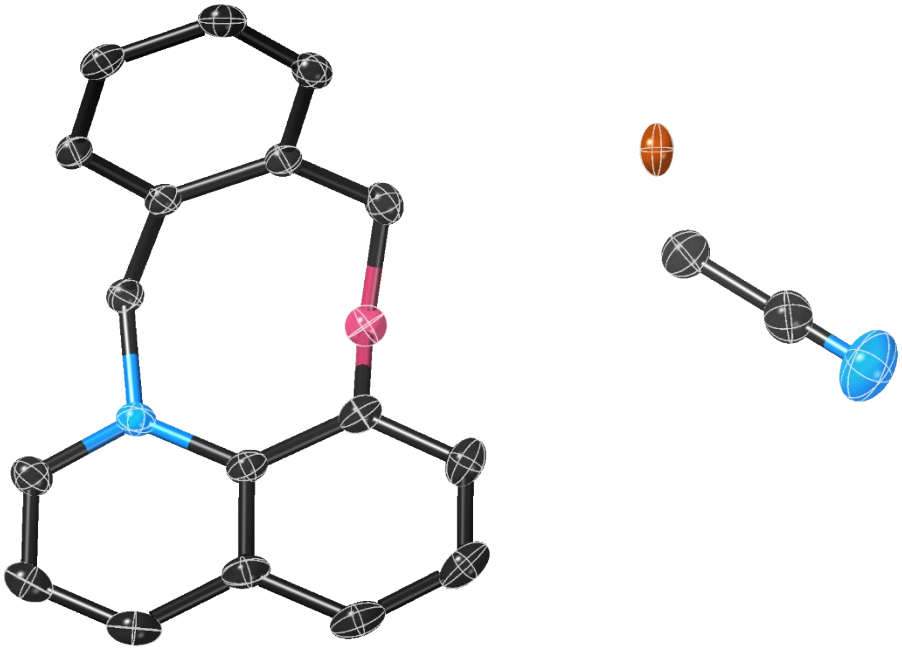

Figure S63. Thermal ellipsoid plot showing the asymmetric unit of **$4\cdot Br\cdot CH_3CN$**.

$DBU^{H}\cdot PF_6$: Small crystals precipitated upon addition of an aqueous solution of NH_4PF_6 to a solution of DBU and $HCl_{(aq)}$. Due to their small size, they required the use of synchrotron radiation.

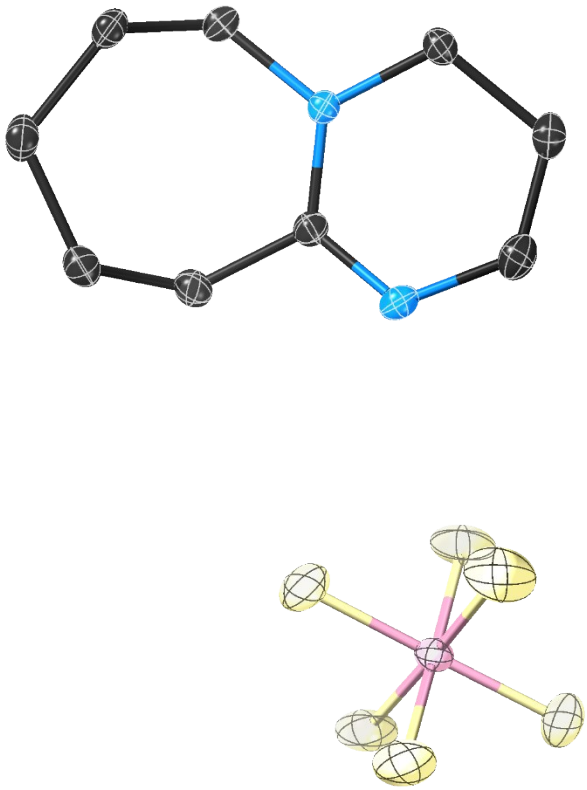

Figure S64. Thermal ellipsoid plot showing the asymmetric unit of $DBU^{H}\cdot PF_6$.

Table of crystallographic data

Table S1. Selected crystallographic data.

Compound	**1·BPh_4**	**1·I**	**2·PF_6·H_2O**	**2·Cl**
Radiation (wavelength)	Cu Kα (1.54184 Å)	Mo Kα (0.71073 Å)	Mo Kα (0.71073 Å)	Cu Kα (1.54184 Å)
Formula	$C_{30}H_{28}BNO$	C_6H_8NOI	$C_{10}H_{12}NO_2F_6P$	$C_{10}H_{10}NOCl$
Formula weight	429.37	237.04	323.17	195.65
a (Å)	16.154(2)	8.1689(2)	6.9715(3)	5.17920(10)
b (Å)	10.0700(15)	30.7155(7)	8.8109(4)	13.1666(3)
c (Å)	14.0816(17)	16.3945(4)	10.7517(4)	6.8217(2)
α (º)	90	90	105.053(4)	90
β (º)	91.992(11)	103.292(3)	99.409(4)	97.057(2)
γ (º)	90	90	94.776(4)	90
Unit cell volume (Å^3)	2289.3(3)	4003.38(10)	623.68(2)	461.664(14)
Crystal system	monoclinic	monoclinic	triclinic	monoclinic
Space group	C_2/m	$P2_1$/c	P–1	$P2_1$
Z	4	20	2	2
Reflections (all)	17202	38419	7730	3222
Reflections (unique)	2302	8122	2549	1755
R_{int}	0.089	0.040	0.021	0.017
R_1 [$I > 2\sigma(I)$]	0.152	0.028	0.042	0.041
$wR_2(F^2)$ (all data)	0.296	0.051	0.102	0.107
CCDC number	2050537	2050536	2050538	2050539

Compound	**2_2·SO_4**	**3·$(PF_6)_2$·C_3H_6O**	**3·$(PF_6)_2$·$(CH_3CN)_3$**
Radiation (wavelength)	Cu Kα (1.54184 Å)	Cu Kα (1.54184 Å)	Cu Kα (1.54184 Å)
Formula	$C_{20}H_{20}N_2O_6S$	$C_{29}H_{28}N_2O_3F_{12}P_2$	$C_{64}H_{62}N_{10}O_4F_{24}P_4$
Formula weight	416.45	742.47	1615.12
a (Å)	7.5285(3)	10.4429(2)	14.8499(5)
b (Å)	17.4636(5)	11.3851(3)	16.5325(6)
c (Å)	6.8720(2)	13.3448(3)	18.0268(7)
α (º)	90	78.042(2)	65.062(4)
β (º)	99.350(3)	78.837(2)	66.010(3)
γ (º)	90	83.599(2)	88.251(3)
Unit cell volume (Å^3)	891.49(3)	1518.60(3)	3612.62(14)
Crystal system	monoclinic	triclinic	triclinic
Space group	$P2_1$/c	P–1	P–1
Z	2	2	2
Reflections (all)	9169	29783	70361
Reflections (unique)	1787	5971	14267
R_{int}	0.051	0.035	0.030
R_1 [$I > 2\sigma(I)$]	0.046	0.057	0.065
$wR_2(F^2)$ (all data)	0.119	0.155	0.187
CCDC number	2050540	2050541	2050542

Compound	**3·Br$_2$**	**3·Cl·PF$_6$·(CH$_3$CN)$_{0.5}$**	**3·Br·PF$_6$·CH$_3$CN**
Radiation (wavelength)	Cu Kα (1.54184 Å)	Cu Kα (1.54184 Å)	Cu Kα (1.54184 Å)
Formula	$C_{26}H_{22}N_2O_2Br_2$	$C_{27}H_{23.5}N_{2.5}O_2F_6PCl$	$C_{28}H_{25}N_3O_2F_6PBr$
Formula weight	554.28	595.41	660.39
a (Å)	7.5194(4)	44.058(12)	14.3441(2)
b (Å)	9.4830(4)	8.6635(3)	11.43670(10)
c (Å)	9.4934(4)	24.582(7)	16.6982(2)
α (°)	118.013(4)	90	90
β (°)	97.791(3)	146.85(6)	90.8455(11)
γ (°)	104.191(4)	90	90
Unit cell volume (Å^3)	553.98(5)	5130.9(15)	2739.03(3)
Crystal system	triclinic	monoclinic	monoclinic
Space group	P-1	C2/c	P2$_1$/c
Z	1	8	4
Reflections (all)	6507	26379	32508
Reflections (unique)	2231	5081	5413
R_{int}	0.013	0.034	0.024
R_1 [$I > 2\sigma(I)$]	0.021	0.046	0.035
$wR_2(F^2)$ (all data)	0.055	0.110	0.081
CCDC number	2050543	2050544	2050545

Compound	**3·SO$_4$·(CH$_3$OH)$_2$**	**3^{-H}·PF$_6$** [a]	**4·Br·CH$_3$CN**	**DBU^H·PF$_6$**
Radiation (wavelength)	synchrotron (0.71073 Å)	Cu Kα (1.54184 Å)	Mo Kα (0.71073 Å)	synchrotron (0.7109 Å)
Formula	$C_{28}H_{30}N_2O_8S$	$C_{26}H_{21}N_2O_2F_6P$·*solvents*	$C_{19}H_{17}N_2OBr$	$C_9H_{17}N_2F_6P$
Formula weight	554.62	538.42	369.26	298.21
a (Å)	7.7620(16)	23.4250(3)	9.8904(2)	6.294(3)
b (Å)	8.7260(17)	23.4250(3)	7.3341(2)	26.438(2)
c (Å)	18.728(4)	18.7771(5)	22.6009(7)	7.670(4)
α (°)	85.64(3)	90	90	90
β (°)	88.48(3)	90	97.141(3)	103.840(10)
γ (°)	89.71(3)	90	90	90
Unit cell volume (Å^3)	1264.3(4)	10303.6(3)	1626.69(5)	1239.24(5)
Crystal system	triclinic	tetragonal	monoclinic	monoclinic
Space group	P-1	I4$_1$/a	P2$_1$/n	P2$_1$/c
Z	2	16	4	4
Reflections (all)	16278	42214	31725	12339
Reflections (unique)	4751	5094	3332	3445
R_{int}	0.172	0.041	0.028	0.021
R_1 [$I > 2\sigma(I)$]	0.126	0.033	0.022	0.035
$wR_2(F^2)$ (all data)	0.219	0.085	0.044	0.087
CCDC number	2050549	2050546	2050547	2050548

[a] PLATON-SQUEEZE[13] used.

pK_a measurements

Rationale for investigating the anion dependence of the pK_a of 2$^+$

The species present when determining the pK_a of **2·Cl** using DBU are shown in Figure S65. There is a strongly favourable interaction between **2**$^+$ and Cl$^-$ (K_a > 10^4 M^{-1} in CD_3CN), while a much weaker interaction between DBU^{H+} and Cl$^-$ would be expected, and we reasoned that this may be sufficient to bias the position of the deprotonation equilibrium. That is, we hypothesized that **2·Cl** would be less prone to deprotonation (*i.e.* less acidic) than **2·BPh$_4$** where no significant hydrogen bond between the O–H group and the anion is expected. In practice, we were not able to conclusively observe any significant difference in the pK_a values (see later).

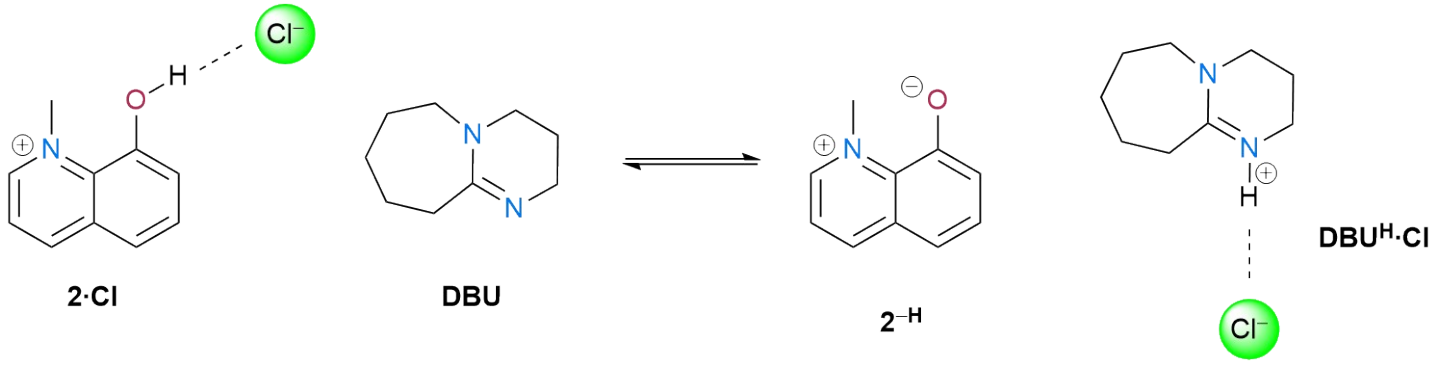

Figure S65. Equilibrium present between **2·Cl** and DBU during pK_a measurements.

To examine this hypothesis further, we prepared DBU^H·PF_6 and measured its chloride recognition properties in CD_3CN (see p13 for synthesis and characterization). The titration protocol was the same as that described in the general protocol (p17). As shown in Figures S66 and 67, a chloride binding constant of 419 M^{-1} was observed, which is significantly less than the very strong binding of chloride to **2·BPh$_4$** observed in the same solvent mixture (K_a > 10^4 M^{-1}), supporting the hypothesis that formation of a hydrogen bond between chloride and **2**$^+$ is preferred over formation of a hydrogen bond between chloride and DBU^{H+}. While clearly there is a difference in solvents used for the chloride binding studies (acetonitrile) and pK_a measurements (DMF), we suggest that based on the similarities in properties between acetonitrile and DMF (*e.g.* almost identical dielectric constants),[14] this experiment still has some relevance.

Anion binding data for DBU^{H}·PF$_6$

Cl$^-$ K_a = 419 M^{-1} ± 5.7% http://app.supramolecular.org/bindfit/view/1a1ae2dd-6138-4887-92b4-4337588c87db

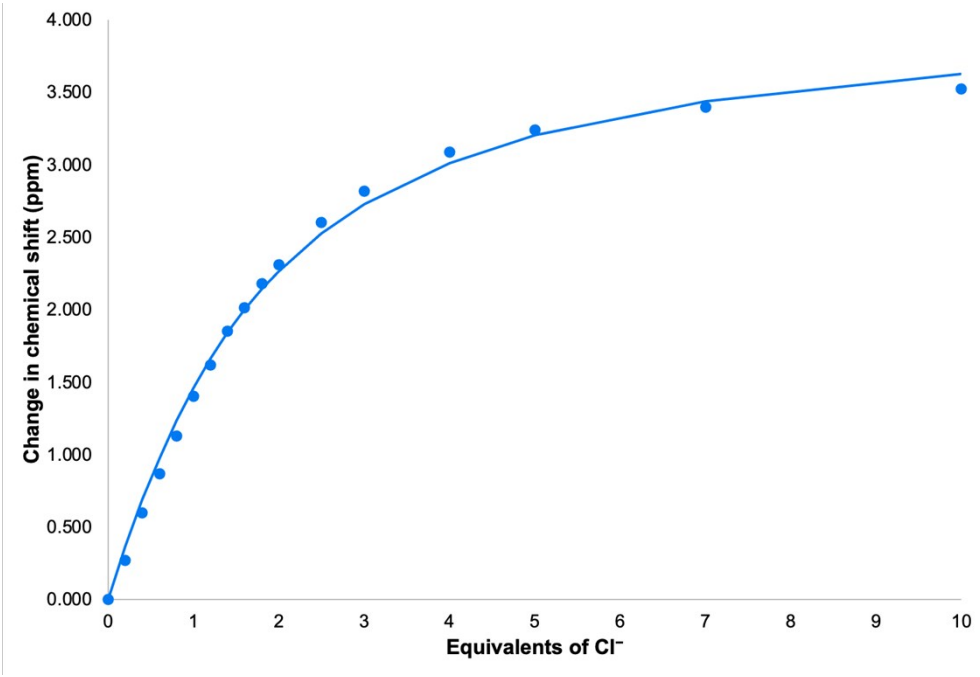

Figure S66. Movement of peak at 7.51 ppm upon addition of TBA·Cl (CD_3CN, 298 K). Points represent observed data, line represents 1:1 isotherm calculated using *Bindfit*.[4]

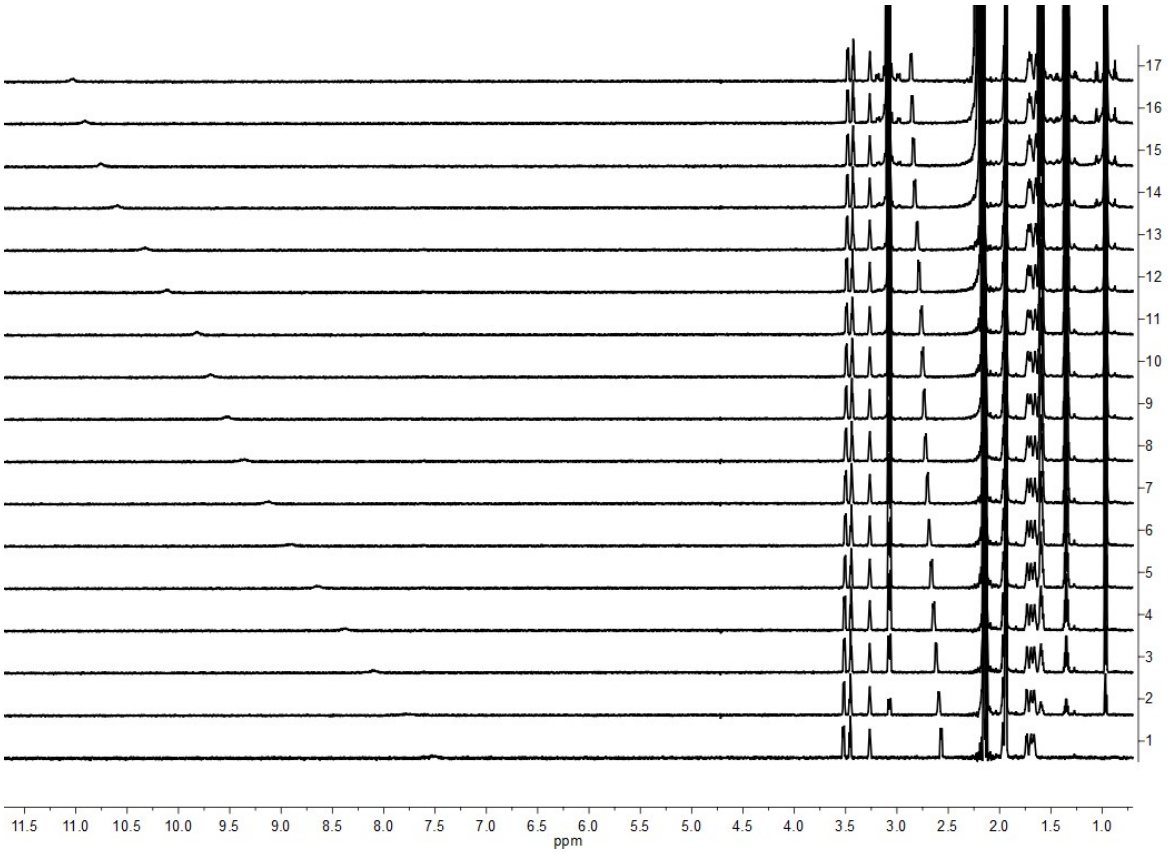

Figure S67. Truncated ^{1}H NMR spectra of DBU^{H}·PF$_6$ upon addition of increasing equivalents of TBA·Cl (CD_3CN, 298 K, 700 MHz).

General remarks for pK_a measurements

Equipment: pH measurements were performed on a Mettler-Toledo SevenCompact S220 pH/ion meter. Titrations in methanol/water were monitored by a Mettler-Toledo InLab Routine ProISM pH probe and those in DMF were monitored by a DGi-116-Solvent pH probe. pH calibrations were carried out using buffered standards at pH 4.01, 7.00 and 9.21. All measurements were carried out four times to allow estimation of errors.

Method, 9:1 MeOH:H_2O: 20 mL solutions of the appropriate salt of $\mathbf{2}^+$ (~ 20–30 mg) were prepared in 9:1 MeOH:H_2O. The liquid level was topped up with additional solvent to ensure that the pH probe was adequately submerged. A 0.01 M sodium hydroxide solution in 9:1 MeOH:H_2O was added to a 25 mL glass burette for titration. Aliquots of this solution were added to a stirred solution of $\mathbf{2}^+$ and the resultant pH recorded after stability was reached. Titration end points were located via the maxima of the first derivative of the resulting titration curve. pK_a values were located according to pH values at titre values corresponding to half of the end point titre. An example titration curve is shown in Figure S68.

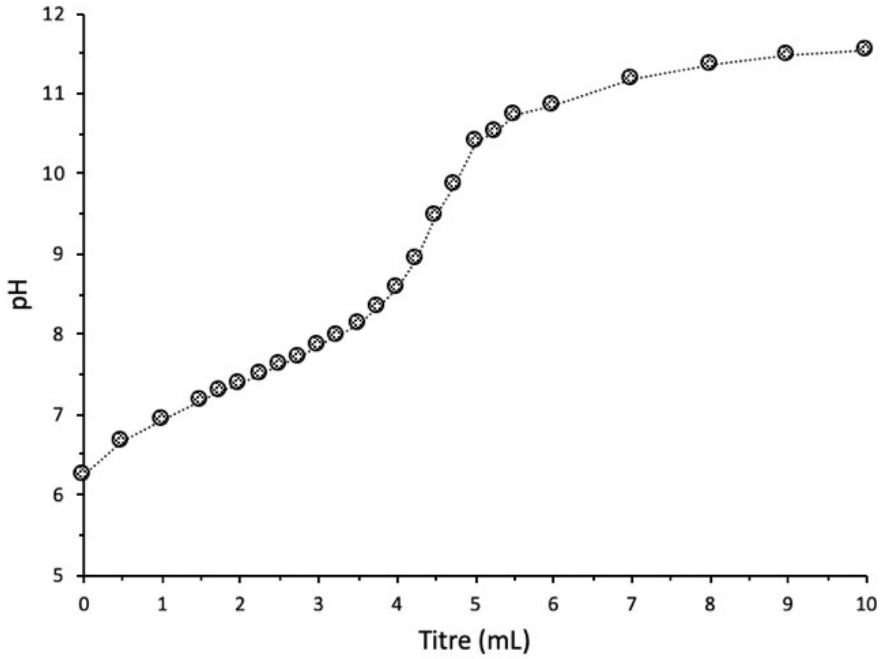

Figure S68. Example pK_a measurement for addition of NaOH to $\mathbf{2{\cdot}BPh_4}$ in 9:1 MeOH:H_2O.

Method, DMF: 20 mL solutions of the appropriate salt of $\mathbf{2}^+$ (~ 35–60 mg) were prepared in DMF. The liquid level was topped up with additional solvent to ensure that the pH probe used was adequately submerged. A ~ 0.02 M DBU solution in DMF was added to a Brand Titrette 25 mL bottle-top burette for titration. Aliquots of this solution were added to a stirred solution of $\mathbf{2}^+$ and the resultant pH recorded after stability was reached. Titration end points were located via the maxima of the first derivative of the resulting titration curve. pK_a values were located according to pH values at titre values corresponding to half of the end point titre.

pK_a measurements for 2·Cl and 2·BPh$_4$

Data for pK_a measurements in 9:1 MeOH:H_2O are provided in Table S2, and in DMF are provided in Table S3. There is no statistically significant difference between the mean values for each anion.

Table S2. pK_a values of **2·Cl** and **2·BPh$_4$** in 9:1 MeOH:H_2O.

	pK_a for 2·Cl	**pK_a for 2·BPh$_4$**
Titration 1	7.47	7.55
Titration 2	7.45	7.56
Titration 3	7.44	7.59
Titration 4	7.38	7.47
Mean	7.44	7.54
95% Confidence interval[a]	7.4 ± 0.1	7.5 ± 0.1

[a] ± 2 standard errors (SE) of the mean, which were estimated as SE = $\sigma/\sqrt{n}$

Table S3. pK_a values of **2·Cl** and **2·BPh$_4$** in DMF.

	pK_a for 2·Cl	**pK_a for 2·BPh$_4$**
Titration 1	9.49	9.56
Titration 2	9.30	9.36
Titration 3	9.60	9.49
Titration 4	9.48	9.43
Mean	9.47	9.46
95% Confidence interval[a]	9.5 ± 0.2	9.5 ± 0.1

[a] ± 2 standard errors (SE) of the mean, which were estimated as SE = $\sigma/\sqrt{n}$

pK_a measurements for "2·PF_6"

As mentioned in the main text of the manuscript, we were able to isolate a crystalline solid by adding $NH_4PF_{6(aq)}$ to a hot concentrated solution of **2·I**. While this gave satisfactory NMR and MS analyses, and was characterised by SCXRD studies, quantitative ^{19}F NMR studies indicated that there was a smaller-than-expected amount of PF_6^- present. We hypothesise that this species is a mixed salt containing a mixture of I^- and PF_6^- anions, and we refer to this compound as **"2·PF_6"** in this section. As shown in Table S4, pK_a measurements of this compound indicate that it is more acidic than **2·Cl** by 0.5 pK_a units, which would fit our initial hypothesis (Figure S65).

We cannot explain why **2·BPh_4** would not also be more acidic than **2·Cl**. While surprisingly short O–H···BPh_4^- interactions have been observed in the solid state,[15] and modest association between aromatic *N*-containing cations and BPh_4^- have been reported,[16] a detailed study has suggested that BPh_4^- is less coordinating than the PF_6^- anion, at least towards metal ions.[17] Given that we know from our solution binding data that Cl^- can readily out-compete the BPh_4^- anion for **2**$^+$'s hydrogen bond, it does not seem plausible that binding of BPh_4^- to **2**$^+$ can explain the lack of difference between pK_a values. Instead, given the uncertainty of the exact composition of **"2·PF_6,"** we are inclined not to trust these results. As a result we have not discussed them in the main text of the manuscript, but include them here for completeness.

Table S4. pK_a values of "**2·PF_6"** in DMF.

	pK_a for "2·PF_6"
Titration 1	9.04
Titration 2	9.04
Titration 3	9.02
Titration 4	8.86
Mean	8.99
95% Confidence interval[a]	9.0 ± 0.1

[a] ± 2 standard errors (SE) of the mean, which were estimated as SE = $\sigma/\sqrt{n}$

Computational studies

Structures and chloride association constants of known receptors in 9:1 CD_3CN:D_2O

Structures of some related molecules are shown in Figure S69. All of these receptors have had their chloride recognition properties measured in 9:1 CD_3CN:D_2O, and these values are provided in the figure. We note that as well as the inherent recognition strength of the motifs used in these receptors, preorganisation effects are likely to play a role – particularly for the larger and more complex host systems.

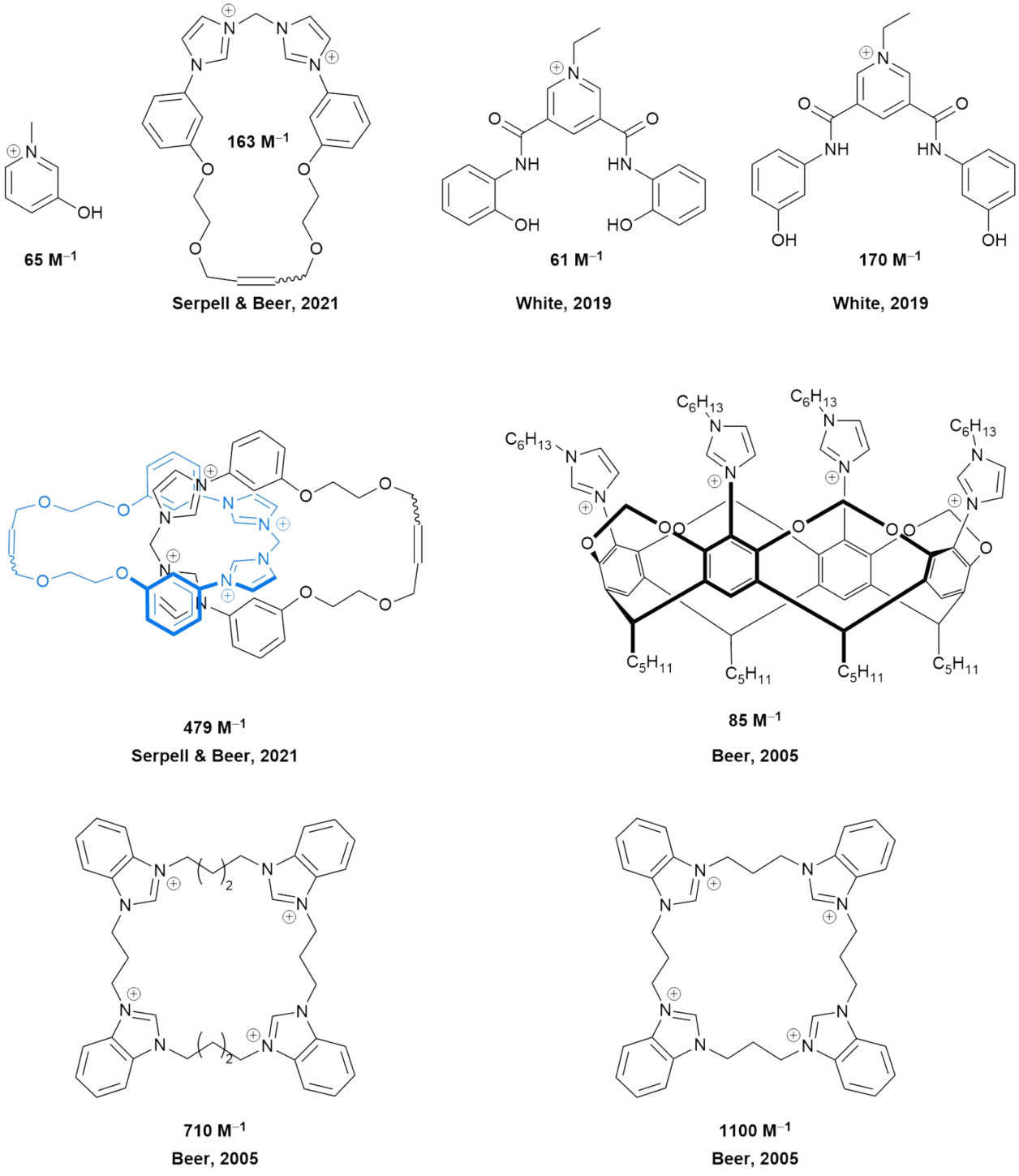

Figure S69. Structures of some anion receptors, and their chloride association constants measured in 9:1 CD_3CN:D_2O. Receptors were reported by Beer in 2005,[18] White in 2019,[19] and Serpell & Beer in 2021.[20]

General protocol

All calculations were performed using the Gaussian 16, Rev. C.01 electronic structure package,[21] except ALMO-EDA(solv) calculations (*vide infra*), at the M06-2X/6-311+G(d,p) level of theory.[22] The nature of all stationary points was confirmed with frequency calculations at the same level. Tight convergence criteria and an Ultrafine grid were used for all species, except nitrocatechol·Cl, where VeryTight criteria and a Superfine grid were used. Gas-phase Gibbs free energies at 298.15 K were calculated using standard textbook formulae based upon the statistical thermodynamics of an ideal gas under the harmonic oscillator and rigid-rotor approximations.

Solvent corrections were obtained with the SMD continuum solvent model,[23] and the thermocycle approach was employed to determine Gibbs free energies in solution.[24] All energies given are from conformationally-searched and Boltzmann-weighted conformer distributions. To prevent possible bias when selecting chloride-binding locations, chloride atoms were randomly distributed around 30 locations in the complex geometries and optimised at the M06-2X/6-31G(d) level; those complexes within 10 kJ mol^{-1} of the lowest energy structure were selected for subsequent refinement at M06-2X/6-311+G(d,p). After this higher level refinement, all conformers within 10 kJ mol^{-1} of the lowest energy structure were used with a Boltzmann weighted average of their energies applied. Solvent calculations were performed either in SMD acetonitrile or in a custom SMD 9:1 MeCN:H_2O solvent defined using interpolated parameters obtained from the SMD models for water and acetonitrile (see Table S18 for details of these parameters).[25]

Interaction energies were determined in SMD solvent with the ALMO-EDA(solv) method[26] implemented in Q-Chem 5.3, using one or both of the SMD models for acetonitrile and the custom CH_3CN:H_2O mixture, where indicated.[27] Briefly, this method partitions the total interaction energy into contributions from preparation, permanent electrostatics, Pauli repulsion, dispersion, polarisation, and charge transfer, while explicitly accounting for solvation. Binding energies were determined with single-point calculations in Q-Chem. Binding energies and interaction energies are counterpoise-corrected.[28] NBO analysis was performed using the Gaussian NBO7 implementation, in the gas-phase.[29] Structures were rendered with Cylview 20,[30] orbital diagrams were rendered with IQmol.[31]

Energy minimized structures and energies

Structures of the lowest energy conformers are provided in Figures S70–S76, as well as Boltzmann weighted Gibbs free energies and components in Tables S5–S11. All energies are provided in Hartrees. The following abbreviations are used.

E(Gas): Total vibrationless energy at 0 K, in the gas-phase; sum of the total electronic energy and nuclear repulsion energy.

ZPVE: Zero point vibrational energy

TC: Thermal correction

G(CP): Counterpoise-corrected Gibbs free energy

E(Soln.): Total vibrationless energy at 0 K, in the SMD solvent field.

G(Soln.): Solution Gibbs free energy

G(Soln.; CP): Counterpoise-corrected solution Gibbs free energy

1·Cl in CH_3CN:

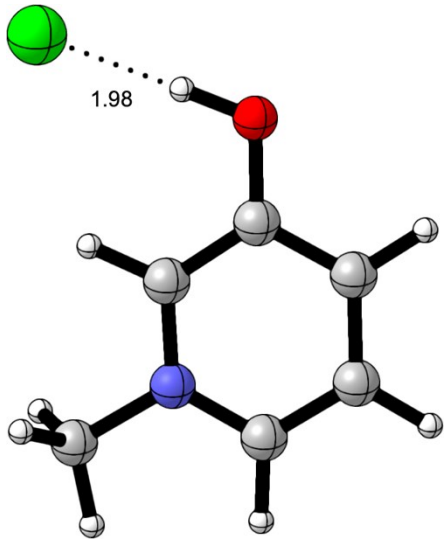

Figure S70. Structure of the lowest energy conformer of **1·Cl** in SMD CH_3CN, distance in Å.

Table S5. Boltzmann weighted Gibbs free energies and components for conformers of **1**$^+$ in SMD CH_3CN.

Species	E(Gas)	ZPVE	TC	TS	H	G	G(CP)	E(Soln.)	G(Soln.)	G(Soln.; CP)	Weighted E(Soln.)	Weighted G(Soln.)	Weighted G(Soln.; CP)
1·Cl	-823.564408	0.129708	0.009990	0.044921	-823.424710	-823.469631	-823.468956	-823.616846	-823.519050	-823.518375	-823.616846	-823.519050	-823.518375
1$^+$ Conf1	-363.126960	0.130645	0.008399	0.039981	-362.987916	-363.027897		-363.224943	-363.122861				
1$^+$ Conf2	-363.128858	0.130596	0.008413	0.040013	-362.989849	-363.029862		-363.225434	-363.123420		-363.2253	-363.1232	
Cl$^-$	-460.268136	0.000000	0.002360	0.017383	-460.265776	-460.283159		-460.373699	-460.385704		-460.373699	-460.385704	

1·Cl in 9:1 CH_3CN:H_2O:

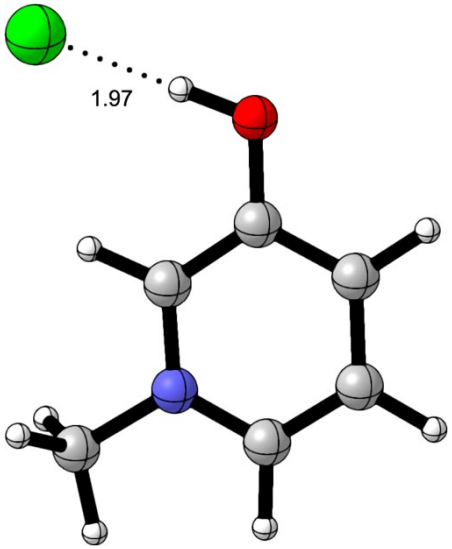

Figure S71. Structure of the lowest energy conformer of **1·Cl** in SMD 9:1 CH_3CN:H_2O, distance in Å.

Table S6. Boltzmann weighted Gibbs free energies and components for conformers of $\mathbf{1^+}$ in SMD 9:1 CH_3CN:H_2O.

Species	E(Gas)	ZPVE	TC	TS	H	G	G(CP)	E(Soln.)	G(Soln.)	G (Soln.; CP)	Weighted E(Soln.)	Weighted G(Soln.)	Weighted G(Soln.; CP)
1·Cl	-823.564408	0.129708	0.009990	0.044921	-823.424710	-823.469631	-823.468956	-823.615612	-823.517816	-823.517138	-823.615612	-823.517816	-823.517138
1^+ Conf1	-363.128858	0.130596	0.008413	0.040013	-362.989849	-363.029862		-363.225664	-363.123649		-363.225664	-363.123649	
Cl^-	-460.268136	0.000000	0.002360	0.017383	-460.265776	-460.283159		-460.3737894	-460.385794		-460.3737894	-460.385794	

2·Cl in CH_3CN:

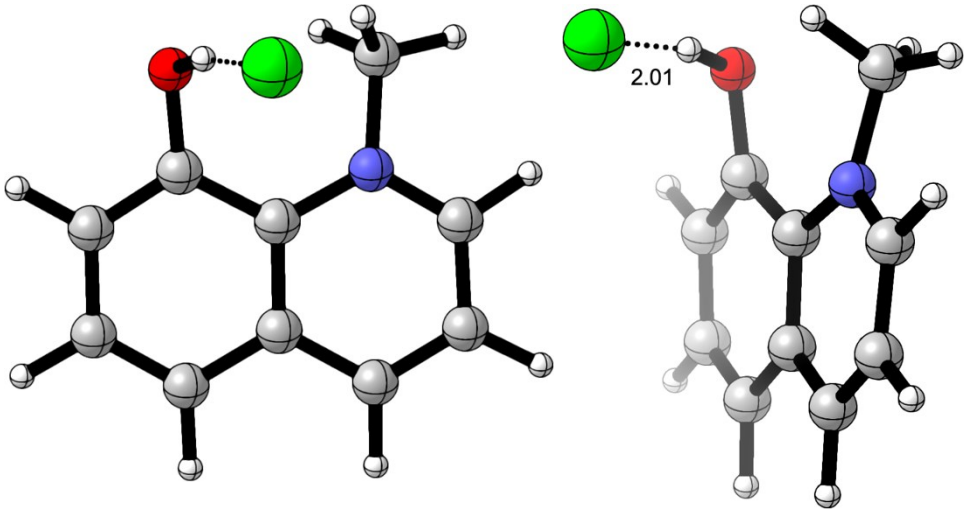

Figure S72. Two views of the structure of the lowest energy conformer of **2·Cl** in SMD CH_3CN, distance in Å.

Table S7. Boltzmann weighted Gibbs free energies and components for conformers of $\mathbf{2^+}$ in SMD CH_3CN.

Species	E(Gas)	ZPVE	TC	TS	H	G	G(CP)	E(Soln.)	G(Soln.)	G (Soln.; CP)	Weighted E(Soln.)	Weighted G(Soln.)	Weighted G(Soln.; CP)
2·Cl	-977.175205	0.175967	0.012316	0.049377	-976.986922	-977.036299	-977.035188	-977.225773	-977.083849	-977.082738	-977.225773	-977.083849	-977.082738
2^+ Conf1	-516.750155	0.176868	0.010764	0.045300	-516.562523	-516.607822		-516.833134	-516.687783		-516.833134	-516.687783	
Cl^-	-460.268136	0.000000	0.002360	0.017383	-460.265776	-460.283159		-460.373699	-460.385704		-460.373699	-460.385704	

Nitrophenol in CH_3CN:

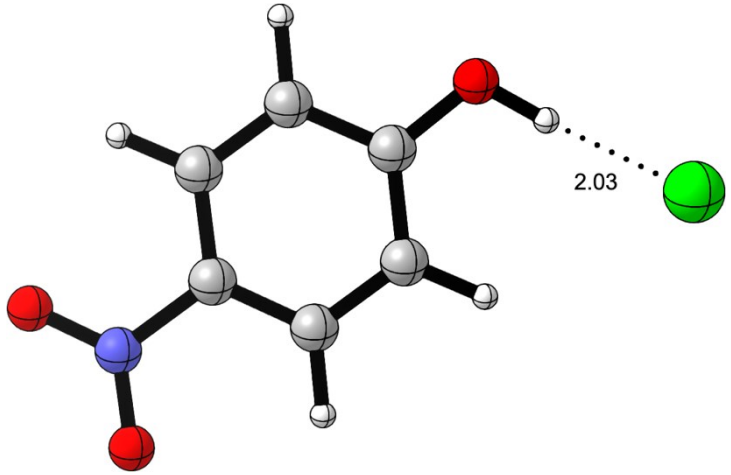

Figure S73. View of the structure of the lowest energy conformer of nitrophenol·Cl in SMD CH_3CN, distance in Å.

Table S8. Boltzmann weighted Gibbs free energies and components for conformers of nitrophenol in SMD CH_3CN.

Species	E(Gas)	ZPVE	TC	TS	H	G	G(CP)	E(Soln.)	G(Soln.)	G (Soln.; CP)	Weighted E(Soln.)	Weighted G(Soln.)	Weighted G(Soln.; CP)
nitrophenol·Cl	-972.239803	0.104484	0.010886	0.047567	-972.124434	-972.172000	-972.171224	-972.320530	-972.249708	-972.248932	-972.320530	-972.249708	-972.248932
nitrophenol Conf1	-511.914710	0.104663	0.009196	0.042456	-511.800852	-511.843308		-511.932942	-511.858522		-511.932942	-511.858522	
Cl^-	-460.268136	0.000000	0.002360	0.017383	-460.265776	-460.283159		-460.373699	-460.385704		-460.373699	-460.385704	

Nitrocatechol in CH_3CN:

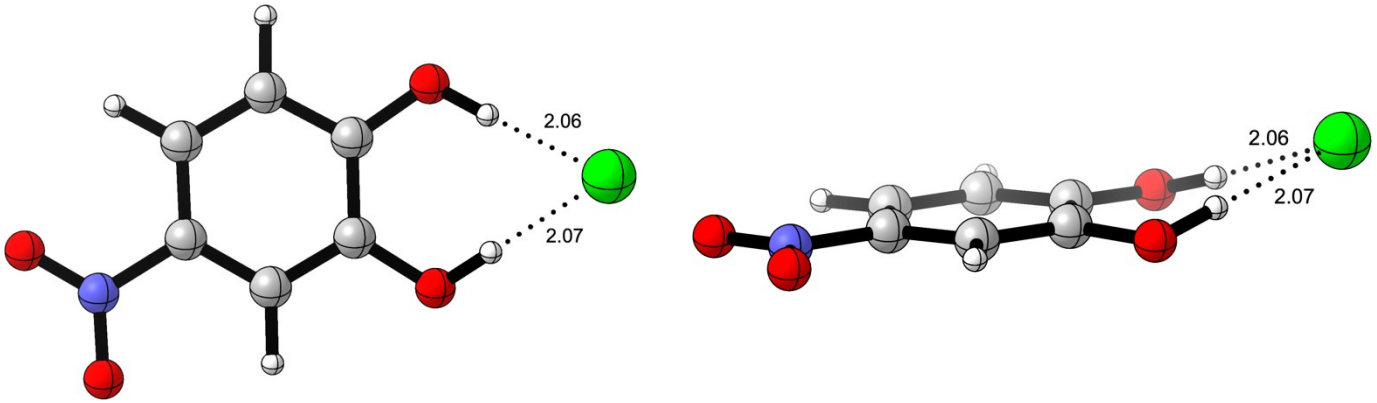

Figure S74. Two views of the structure of the lowest energy conformer of nitrocatechol·Cl in SMD CH_3CN, distance in Å.

Table S9. Boltzmann weighted Gibbs free energies and components for conformers of nitrocatechol in SMD CH_3CN.

Species	E(Gas)	ZPVE	TC	TS	H	G	G(CP)	E(Soln.)	G(Soln.)	G (Soln.; CP)	Weighted E(Soln.)	Weighted G(Soln.)	Weighted G(Soln.; CP)
nitrocatechol·Cl	-1047.474122	0.108498	0.011886	0.049408	-1047.353738	-1047.403146	-1047.402373	-1047.548715	-1047.474721	-1047.473947	-1047.548715	-1047.474721	-1047.473947
nitrocatechol Conf1	-587.139570	0.108681	0.010586	0.045418	-587.020303	-587.065722		-587.159225	-587.082358				
nitrocatechol Conf2	-587.140839	0.108820	0.010547	0.045355	-587.021473	-587.066828		-587.159512	-587.082482		-587.159390	-587.082424	
Cl^-	-460.268136	0.000000	0.002360	0.017383	-460.265776	-460.283159		-460.373699	-460.385704		-460.373699	-460.385704	

4·Cl in CH_3CN:

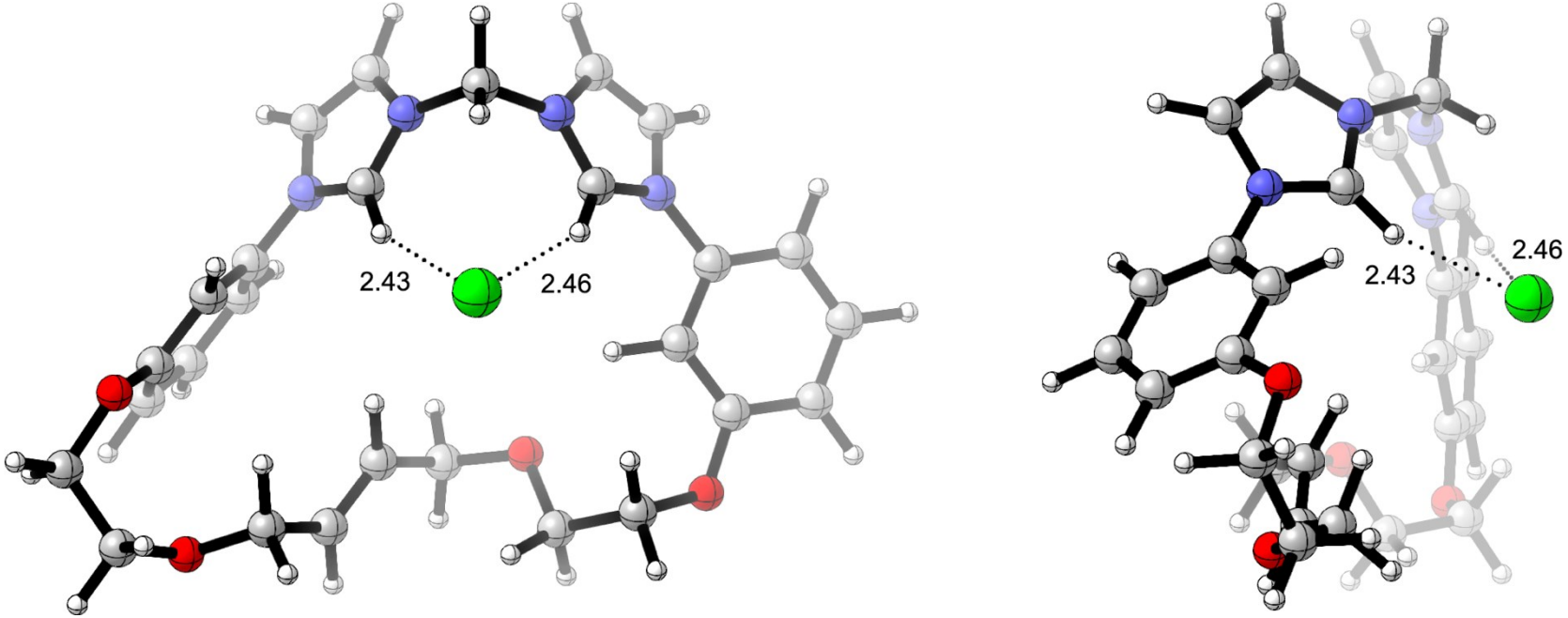

Figure S75. Two views of the structure of the lowest energy conformer of **4·Cl** in SMD CH_3CN, distances in Å.

Table S10. Boltzmann weighted Gibbs free energies and components for conformers of **4·Cl** in SMD CH_3CN.

Species	E(Gas)	ZPVE	TC	TS	H	G	G(CP)	E(Soln.)	G(Soln.)	G (Soln.; CP)	Weighted E(Soln.)	Weighted G(Soln.)	Weighted G(Soln.; CP)
4·Cl Conf1	-2026.545733	0.528393	0.033158	0.093312	-2025.984182	-2026.077495	-2026.076130	-2026.679408	-2026.208151	-2026.206786			
4·Cl Conf2	-2026.546176	0.529283	0.033119	0.093264	-2025.983774	-2026.077038	-2026.075626	-2026.678029	-2026.205872	-2026.204460	-2026.679148	-2026.207964	-2026.206604
4^{2+} Conf1	-1566.007616	0.527936	0.031374	0.089549	-1565.448306	-1565.537855		-1566.287621	-1565.814841				
4^{2+} Conf2	-1566.007371	0.527786	0.031558	0.090208	-1565.448027	-1565.538235		-1566.286584	-1565.814429				
4^{2+} Conf3	-1566.010116	0.528176	0.031249	0.089201	-1565.45069	-1565.539891		-1566.285396	-1565.812152				
4^{2+} Conf4	-1566.012583	0.528522	0.030977	0.088296	-1565.453085	-1565.541381		-1566.288859	-1565.814638				
4^{2+} Conf5	-1566.011281	0.528119	0.03143	0.089769	-1565.451731	-1565.541501		-1566.288486	-1565.815687		-1566.288433	-1565.815141	
Cl^-	-460.268136	0.000000	0.002360	0.017383	-460.265776	-460.283159		-460.373699	-460.385704		-460.373699	-460.385704	

4·Cl in 9:1 CH_3CN:H_2O:

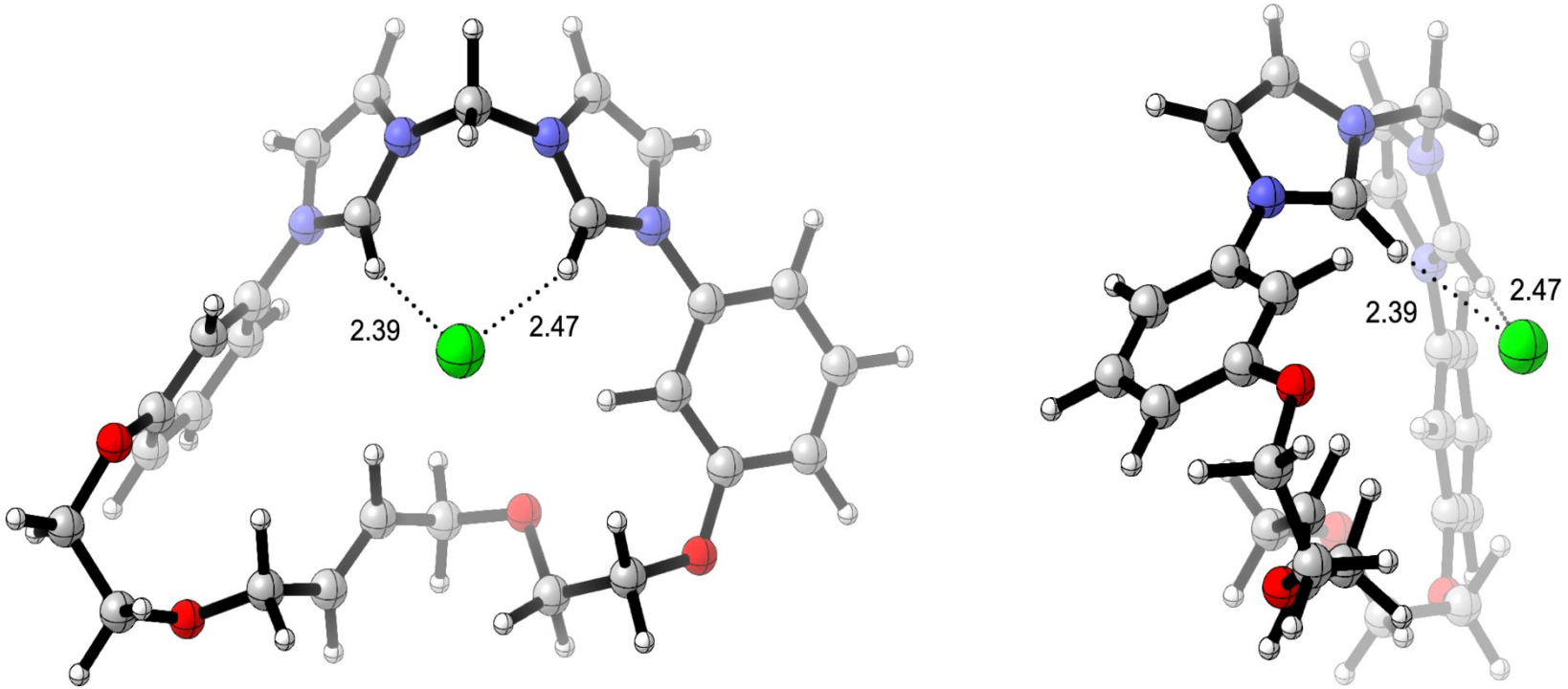

Figure S76. Two views of the structure of the lowest energy conformer of **4·Cl** in SMD 9:1 CH_3CN:H_2O, distances in Å.

Table S11. Boltzmann weighted Gibbs free energies and components for conformers of **4·Cl** in SMD 9:1 CH_3CN:H_2O.

Species	E(Gas)	ZPVE	TC	TS	H	G	G(CP)	E(Soln.)	G(Soln.)	G (Soln.; CP)	Weighted E(Soln.)	Weighted G(Soln.)	Weighted G(Soln.; CP)
4·Cl Conf1	-2026.545733	0.528393	0.033158	0.093312	-2025.984182	-2026.077495	-2026.076051	-2026.676008	-2026.204751	-2026.203307			
4·Cl Conf2	-2026.546176	0.529283	0.033119	0.093264	-2025.983774	-2026.077038	-2026.075520	-2026.674527	-2026.202370	-2026.200853	-2026.675753	-2026.204574	-2026.203137
4^{2+} Conf1	-1566.007616	0.527936	0.031374	0.089549	-1565.448306	-1565.537855		-1566.284534	-1565.811754				
4^{2+} Conf2	-1566.007371	0.527786	0.031558	0.090208	-1565.448027	-1565.538235		-1566.283485	-1565.811330				
4^{2+} Conf3	-1566.012583	0.528522	0.030977	0.088296	-1565.453085	-1565.541381		-1566.285961	-1565.811740				
4^{2+} Conf4	-1566.011281	0.528119	0.031430	0.089769	-1565.451731	-1565.541501		-1566.285191	-1565.812392		-1566.285480	-1565.811966	
Cl^-	-460.268136	0.000000	0.002360	0.017383	-460.265776	-460.283159		-460.373699	-460.385704		-460.373699	-460.385704	

ALMO-EDA(solv) interaction energies in CH_3CN and 9:1 $CH_3CN:H_2O$

Boltzmann weighted ALMO-EDA(solv) interaction energies and their components are presented in Figure S77 and Table S12. Note that these are the same data presented in Figure 6 of the main manuscript with the addition of values for **1·Cl** and **4·Cl** in 9:1 $CH_3CN:H_2O$.

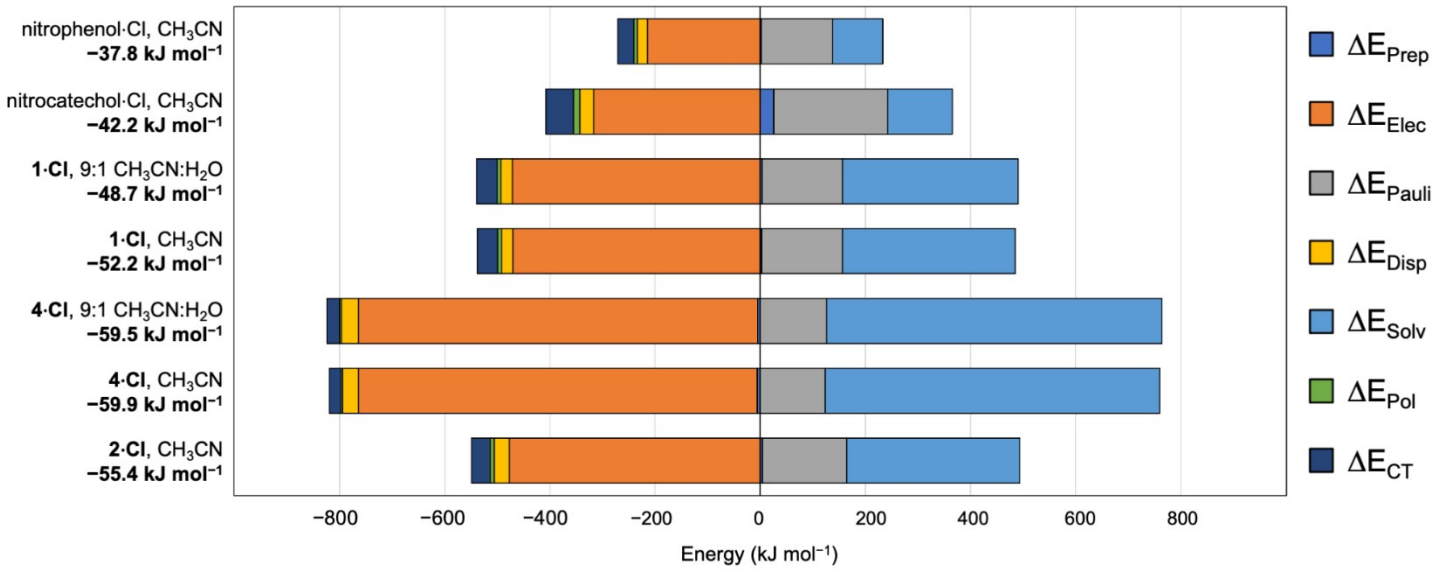

Figure S77. Boltzmann weighted ALMO-EDA(solv) interaction energies and their components for each studied species. Overall interaction energies are given in bold next to the compound name.

Table S12. Boltzmann weighted ALMO-EDA(solv) interaction energies and components for conformers of each studied molecule. Energies are in kJ/mol. Geometries used were taken from solvent calculations.

Species	ΔE_{Prep}	ΔE_{Elec}	ΔE_{Pauli}	ΔE_{Disp}	ΔE_{Solv}	ΔE_{Pol}	ΔE_{CT}	ΔE_{Int}	$\Delta E_{Binding}$
1·Cl (CH_3CN)	2.9732	-470.5507	153.2828	-21.2851	329.4422	-7.5341	-38.5479	-52.2196	-52.8877
1·Cl (9:1 $CH_3CN:H_2O$)	3.2927	-471.6551	153.0028	-21.2281	334.2847	-7.0712	-39.2827	-48.6569	-49.3931
2·Cl	3.9200	-476.7008	160.3687	-29.3417	329.7450	-7.2303	-36.1361	-55.3752	-56.1208
nitrophenol·Cl	2.1086	-213.8781	135.3113	-19.7008	95.4803	-6.0845	-30.9961	-37.7593	-38.4772
nitrocatechol·Cl	26.0619	-316.3491	215.9698	-26.3082	123.4558	-12.4630	-52.6168	-42.2496	-43.3206
4·Cl (CH_3CN)	-5.8098	-757.8585	123.4429	-30.2499	636.3261	-3.4414	-22.2644	-59.8551	-57.5279
4·Cl (9:1 $CH_3CN:H_2O$)	-4.8399	-758.9591	126.4898	-32.4486	637.6408	-3.5184	-23.8208	-59.4561	-56.4903

Abbreviations used: Prep = preparative, Elec = electrostatic, Pauli = Pauli repulsion, Disp = dispersion, Solv = solvation, Pol = polarisation, CT = charge transfer, Int = interaction.

NBO analysis of interactions

Estimates for the second order donor–acceptor interactions in the NBO basis for **1·Cl** (in CH_3CN and 9:1 CH_3CN), and **2·Cl**, nitrophenol·Cl and nitrocatechol·Cl (in CH_3CN) are presented in Tables S13–S17. Only interactions where the donor resides on the chloride anion are shown.

Table S13. Second order perturbative estimates of donor–acceptor interactions in the NBO basis of **1·Cl** in CH_3CN.

Donor NBO	Acceptor NBO	E(2) (kJ mol^{-1})
16. LP(1) Cl17	53. BD*(1) C6-H12	0.418
16. LP(1) Cl17	**57. BD*(1) O8-H16**	**9.498**
16. LP(1) Cl17	229. RY(1) H16	0.502
16. LP(1) Cl17	233. RY(5) H16	0.209
17. LP(2) Cl17	51. BD*(2) C5-C6	0.377
17. LP(2) Cl17	145. RY(3) C6	0.209
17. LP(2) Cl17	231. RY(3) H16	0.418
18. LP(3) Cl17	41. BD*(1) N1-C6	0.628
18. LP(3) Cl17	53. BD*(1) C6-H12	7.155
18. LP(3) Cl17	144. RY(2) C6	0.335
18. LP(3) Cl17	209. RY(1) H12	0.251
19. LP(4) Cl17	41. BD*(1) N1-C6	0.669
19. LP(4) Cl17	52. BD*(1) C5-O8	0.335
19. LP(4) Cl17	53. BD*(1) C6-H12	1.925
19. LP(4) Cl17	**57. BD*(1) O8-H16**	**181.544**
19. LP(4) Cl17	126. RY(1) C5	0.418
19. LP(4) Cl17	178. RY(2) O8	1.799
19. LP(4) Cl17	179. RY(3) O8	0.251
19. LP(4) Cl17	191. RY(15) O8	0.251
19. LP(4) Cl17	192. RY(16) O8	0.418
19. LP(4) Cl17	229. RY(1) H16	2.887
19. LP(4) Cl17	230. RY(2) H16	0.586
19. LP(4) Cl17	232. RY(4) H16	0.586
19. LP(4) Cl17	233. RY(5) H16	1.632
	Total Interactions	213.300
	Explained by LP Cl^- → BD* O–H	**89.6%**

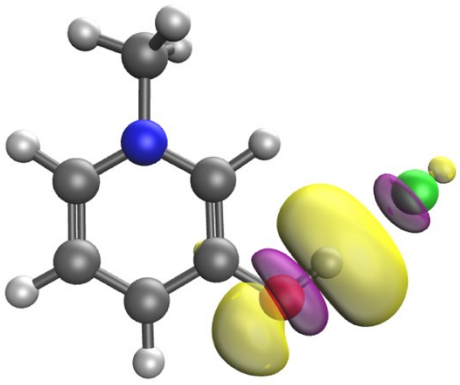

Figure S78. O-H antibonding orbital identified as major contributor to interaction energy in **Table S13**. Isovalue of 0.07 was chosen aesthetically.

Table S14. Second order perturbative estimates of donor–acceptor interactions in the NBO basis of **1·Cl** in 9:1 CH_3CN:H_2O.

Donor NBO	Acceptor NBO	E(2) (kJ mol^{-1})
16. LP (1) Cl17	53. BD*(1) C6-H12	0.460
16. LP (1) Cl17	**57. BD*(1) O8-H16**	**9.372**
16. LP (1) Cl17	229. RY(1) H16	0.502
17. LP (2) Cl17	51. BD*(2) C5-C6	0.377
17. LP (2) Cl17	145. RY(3) C6	0.209
17. LP (2) Cl17	231. RY(3) H16	0.377
18. LP (3) Cl17	41. BD*(1) N1-C6	0.669
18. LP (3) Cl17	53. BD*(1) C6-H12	7.322
18. LP (3) Cl17	144. RY(2) C6	0.335
18. LP (3) Cl17	209. RY(1) H12	0.251
19. LP (4) Cl17	41. BD*(1) N1-C6	0.669
19. LP (4) Cl17	52. BD*(1) C5-O8	0.335
19. LP (4) Cl17	53. BD*(1) C6-H12	1.966
19. LP (4) Cl17	**57. BD*(1) O8-H16**	**179.494**
19. LP (4) Cl17	126. RY(1) C5	0.418
19. LP (4) Cl17	178. RY(2) O8	1.757
19. LP (4) Cl17	179. RY(3) O8	0.293
19. LP (4) Cl17	191. RY(15) O8	0.251
19. LP (4) Cl17	192. RY(16) O8	0.418
19. LP (4) Cl17	229. RY(1) H16	2.845
19. LP (4) Cl17	230. RY(2) H16	0.586
19. LP (4) Cl17	232. RY(4) H16	0.544
19. LP (4) Cl17	233. RY(5) H16	1.674
	Total Interactions	211.125
	Explained by LP Cl^- → BD* O–H	**89.5%**

Table S15. Second order perturbative estimates of donor–acceptor interactions in the NBO basis of **2·Cl** in CH_3CN.

Donor NBO	Acceptor NBO	E(2) (kJ mol^{-1})
20. LP(1) Cl23	77. BD*(1) C11-H20	0.377
20. LP(1) Cl23	**79. BD*(1) O12-H22**	**8.954**
20. LP(1) Cl23	328. RY(1) H22	0.460
21. LP(2) Cl23	64. BD*(2) C5-C6	0.502
21. LP(2) Cl23	68. BD*(2) C7-C8	0.837
21. LP(2) Cl23	77. BD*(1) C11-H20	1.046
22. LP(3) Cl23	64. BD*(2) C5-C6	0.209
22. LP(3) Cl23	77. BD*(1) C11-H20	5.648
22. LP(3) Cl23	**79. BD*(1) O12-H22**	0.418
22. LP(3) Cl23	329. RY(2) H22	0.251
23. LP(4) Cl23	53. BD*(2) N1-C2	0.251
23. LP(4) Cl23	64. BD*(2) C5-C6	0.544
23. LP(4) Cl23	68. BD*(2) C7-C8	0.544
23. LP(4) Cl23	69. BD*(1) C7-O12	0.418
23. LP(4) Cl23	77. BD*(1) C11-H20	3.054
23. LP(4) Cl23	**79. BD*(1) O12-H22**	**158.239**
23. LP(4) Cl23	182. RY(1) C7	0.460
23. LP(4) Cl23	267. RY(2) O12	1.046
23. LP(4) Cl23	271. RY(6) O12	0.920
23. LP(4) Cl23	318. RY(1) H20	0.209
23. LP(4) Cl23	328. RY(1) H22	2.050
23. LP(4) Cl23	330. RY(3) H22	0.920
23. LP(4) Cl23	331. RY(4) H22	0.418
23. LP(4) Cl23	332. RY(5) H22	1.423
	Total Interactions	189.200
	Explained by LP Cl^- → BD* O–H	**88.4%**

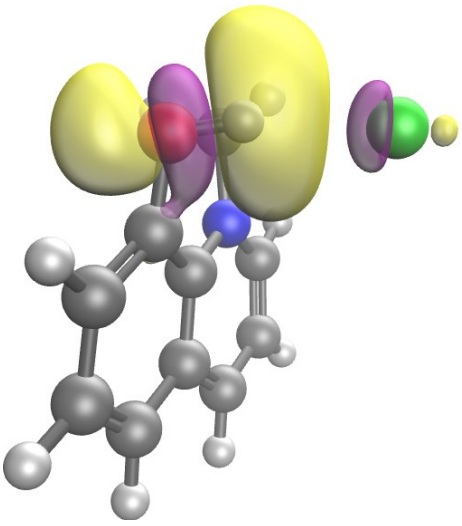

Figure S79. O-H antibonding orbital identified as major contributor to interaction energy in **Table S15**. Isovalue of 0.07 was chosen aesthetically.

Table S16. Second order perturbative estimates of donor–acceptor interactions in the NBO basis of nitrophenol·Cl in CH_3CN.

Donor NBO	Acceptor NBO	E(2) (kJ mol^{-1})
23. LP(1) Cl16	**61. BD*(1) O7-H15**	**6.653**
23. LP(1) Cl16	255. RY(1) H15	0.377
24. LP(2) Cl16	51. BD*(2) C2-C3	0.251
24. LP(2) Cl16	256. RY(2) H15	0.251
25. LP(3) Cl16	50. BD*(1) C2-C3	0.335
25. LP(3) Cl16	52. BD*(1) C2-H11	3.891
26. LP(4) Cl16	49. BD*(1) C1-O7	0.335
26. LP(4) Cl16	50. BD*(1) C2-C3	0.251
26. LP(4) Cl16	52. BD*(1) C2-H11	1.255
26. LP(4) Cl16	**61. BD*(1) O7-H15**	**138.741**
26. LP(4) Cl16	65. RY(1) C1	0.418
26. LP(4) Cl16	168. RY(2) O7	0.460
26. LP(4) Cl16	169. RY(3) O7	1.297
26. LP(4) Cl16	170. RY(4) O7	0.209
26. LP(4) Cl16	176. RY(10) O7	0.293
26. LP(4) Cl16	182. RY(16) O7	0.293
26. LP(4) Cl16	235. RY(1) H11	0.251
26. LP(4) Cl16	255. RY(1) H15	1.757
26. LP(4) Cl16	257. RY(3) H15	0.377
26. LP(4) Cl16	258. RY(4) H15	0.293
26. LP(4) Cl16	259. RY(5) H15	1.674
	Total Interactions	159.661
	Explained by LP Cl^- → BD* O-H	**91.1%**

Table S17. Second order perturbative estimates of donor–acceptor interactions in the NBO basis of nitrocatechol·Cl in CH_3CN.

Donor NBO	Acceptor NBO	E(2) (kJ mol^{-1})
26. LP(1) Cl17	**65. BD*(1) O7-H15**	**4.268**
26. LP(1) Cl17	**66. BD*(1) O8-H16**	**3.975**
27. LP(2) Cl17	**65. BD*(1) O7-H15**	**1.464**
27. LP(2) Cl17	**66. BD*(1) O8-H16**	**1.339**
28. LP(3) Cl17	53. BD*(1) C1-O7	0.251
28. LP(3) Cl17	64. BD*(1) C6-O8	0.251
28. LP(3) Cl17	**65. BD*(1) O7-H15**	**22.175**
28. LP(3) Cl17	**66. BD*(1) O8-H16**	**25.104**
28. LP(3) Cl17	174. RY(3) O7	0.251
28. LP(3) Cl17	191. RY(3) O8	0.209
28. LP(3) Cl17	272. RY(1) H15	0.460
28. LP(3) Cl17	276. RY(5) H15	0.293
28. LP(3) Cl17	277. RY(1) H16	0.460
28. LP(3) Cl17	281. RY(5) H16	0.335
29. LP(4) Cl17	**65. BD*(1) O7-H15**	**88.994**
29. LP(4) Cl17	**66. BD*(1) O8-H16**	**80.960**
29. LP(4) Cl17	174. RY(3) O7	0.628
29. LP(4) Cl17	191. RY(3) O8	0.502
29. LP(4) Cl17	272. RY(1) H15	0.669
29. LP(4) Cl17	274. RY(3) H15	0.209
29. LP(4) Cl17	276. RY(5) H15	1.381
29. LP(4) Cl17	277. RY(1) H16	0.544
29. LP(4) Cl17	281. RY(5) H16	1.297
	Total Interactions	236.019
	Explained by LP Cl^- → BD* O–H	**96.7%**

Table S18. Parameters defining the SMD models of water and acetonitrile, and the interpolated custom 9:1 CH_3CN:H_2O. Parameters were taken from the Supporting Information of Ref. 25.

Parameter	SMD Acetonitrile	SMD Water	9:1 CH_3CN:H_2O
Dielectric constant[a]	35.68	78.355	39.95
Refractive index[b]	1.34	1.3328	1.343
Bulk surface tension[c]	41.25	103.62	47.487
Abraham acidity[d]	0.07	0.82	0.145
Abraham basicity[e]	0.32	0.35	0.323
Carbon aromaticity[f]	0.00	n.a. (0.00)[h]	0.00
Electronegative halogenicity[g]	0.00	n.a. (0.00)[h]	0.00

[a] Dielectric constant at 298.15 K. [b] Index of refraction at optical frequencies at 293 K. [c] Macroscopic surface tension in cal mol^{-1} $Å^2$. [d] Abraham's hydrogen bond acidity parameter. [e] Abraham's hydrogen bond basicity parameter. [f] Fraction of non-hydrogenic solvent atoms that are aromatic carbon atoms. [g] Fraction of non-hydrogenic atoms in the solvent molecule that are F, Cl, or Br. [h] Values are not defined in the SMD model, and are taken to be zero.

Atomic coordinates

1·Cl, gas phase

N	0.13462	0.10884	1.06582
C	-0.18010	-1.19530	1.19251
C	-0.30839	-1.96845	0.05509
C	-0.11730	-1.40614	-1.19550
C	0.20967	-0.04489	-1.31804
C	0.33134	0.69424	-0.12310
C	0.32403	0.92704	2.27838
O	0.38580	0.48872	-2.48979
H	-0.31661	-1.56985	2.19613
H	-0.56382	-3.01427	0.15974
H	-0.21703	-1.99233	-2.10059
H	0.58300	1.75072	-0.15134
H	-0.33668	0.55943	3.05987
H	0.08259	1.96033	2.04282
H	1.36314	0.85367	2.59710
H	0.61141	1.51632	-2.41046
Cl	0.96158	3.20732	-1.94753

1·Cl, CH_3CN

N	0.13770	0.08595	1.09643
C	-0.21442	-1.20250	1.19792
C	-0.36379	-1.96395	0.05062
C	-0.14944	-1.39203	-1.18818
C	0.21808	-0.04366	-1.27415
C	0.35507	0.67780	-0.09297
C	0.30106	0.91117	2.31087
O	0.42170	0.49556	-2.47319
H	-0.36752	-1.59067	2.19419
H	-0.64836	-3.00304	0.14512
H	-0.26003	-1.96694	-2.10020
H	0.63621	1.72362	-0.07795
H	0.09305	0.29848	3.18298
H	-0.39722	1.74446	2.25753
H	1.32486	1.27957	2.34182
H	0.67773	1.45869	-2.40931
Cl	1.18258	3.36288	-2.25044

1^+, Conf1, gas phase

N	0.15060	0.10725	1.08037
C	-0.22490	-1.17371	1.18272
C	-0.37903	-1.94412	0.03899
C	-0.14436	-1.38598	-1.20029
C	0.24818	-0.04307	-1.28845
C	0.38836	0.68464	-0.11720
C	0.31776	0.93785	2.29508
O	0.46475	0.45703	-2.50442
H	-0.39433	-1.55561	2.17945
H	-0.68292	-2.97736	0.13840
H	-0.25421	-1.95565	-2.11558
H	0.68756	1.72551	-0.10033
H	0.09188	0.33271	3.16820
H	-0.36903	1.78089	2.24170
H	1.34792	1.28666	2.34338
H	0.73153	1.38326	-2.49736

1^+, Conf1, CH_3CN

N	0.13583	0.11357	1.07207
C	-0.20210	-1.17778	1.18287
C	-0.34003	-1.95453	0.04509
C	-0.12721	-1.39408	-1.19985
C	0.22492	-0.04622	-1.28779
C	0.35078	0.69324	-0.12319
C	0.32279	0.93363	2.28713
O	0.42653	0.48273	-2.50613
H	-0.35425	-1.55704	2.18307
H	-0.61564	-2.99494	0.15017
H	-0.22967	-1.97701	-2.10743
H	0.62034	1.74302	-0.11520
H	-0.15059	0.42660	3.12264
H	-0.13798	1.90495	2.12226
H	1.39154	1.04541	2.46444
H	0.66451	1.41875	-2.44551

1^+, Conf2, gas phase

N	0.14093	0.09986	1.05548
C	-0.20629	-1.19223	1.19068
C	-0.33738	-1.98993	0.06956
C	-0.11046	-1.45778	-1.18966
C	0.25067	-0.11424	-1.30675
C	0.36903	0.64725	-0.14865
C	0.32138	0.94349	2.26000
O	0.49590	0.52290	-2.45177
H	-0.37008	-1.55155	2.19663
H	-0.61999	-3.02679	0.19194
H	-0.21357	-2.07647	-2.07463
H	0.64668	1.69249	-0.18738
H	-0.22400	0.49541	3.08597
H	-0.07280	1.93603	2.05533
H	1.38374	0.99706	2.49461
H	0.39683	-0.04781	-3.22271

1^+, Conf2, CH_3CN

N	0.13884	0.10264	1.05496
C	-0.20927	-1.18685	1.18813
C	-0.33771	-1.98288	0.06602
C	-0.10673	-1.44791	-1.18997
C	0.25317	-0.10534	-1.29925
C	0.37017	0.65593	-0.14584
C	0.32013	0.93941	2.25956
O	0.49769	0.51706	-2.46471
H	-0.37566	-1.54424	2.19402
H	-0.62063	-3.01974	0.18585
H	-0.20543	-2.05996	-2.07984
H	0.64635	1.70187	-0.16592
H	-0.20903	0.47389	3.08577
H	-0.08526	1.92805	2.05814
H	1.38565	1.00236	2.47614
H	0.38831	-0.09661	-3.20442

1·Cl, 9:1 CH_3CN:H_2O

N	0.13945	0.08526	1.09715
C	-0.21266	-1.20329	1.19814
C	-0.36431	-1.96380	0.05063
C	-0.15216	-1.39074	-1.18804
C	0.21534	-0.04271	-1.27308
C	0.35471	0.67805	-0.09223
C	0.30501	0.90943	2.31200
O	0.41704	0.49803	-2.47298
H	-0.36389	-1.59231	2.19437
H	-0.64887	-3.00291	0.14477
H	-0.26432	-1.96402	-2.10077
H	0.63598	1.72383	-0.07691
H	0.09937	0.29568	3.18390
H	-0.39402	1.74224	2.26129
H	1.32857	1.27856	2.34114
H	0.67351	1.46143	-2.40857
Cl	1.17851	3.36270	-2.25970

1^+, Conf1, 9:1 CH_3CN:H_2O

N	0.14772	0.09707	1.07888
C	-0.22779	-1.18418	1.18118
C	-0.38100	-1.95135	0.03825
C	-0.14579	-1.39160	-1.20262
C	0.24478	-0.05342	-1.28208
C	0.38538	0.67543	-0.11304
C	0.31472	0.92627	2.29057
O	0.46979	0.47661	-2.49552
H	-0.39711	-1.56589	2.17730
H	-0.68479	-2.98448	0.13748
H	-0.25765	-1.96751	-2.11356
H	0.68488	1.71647	-0.10174
H	0.08822	0.32078	3.16326
H	-0.36927	1.77048	2.22587
H	1.34468	1.27629	2.32783
H	0.73365	1.40627	-2.42521

2·Cl, gas phase

N	-0.08015	0.88276	1.11642
C	-0.32892	0.25153	2.25199
C	-0.46261	-1.13692	2.32423
C	-0.23767	-1.86953	1.19035
C	0.00397	-1.22440	-0.04210
C	-0.03538	0.19686	-0.08474
C	-0.04601	0.86528	-1.35026
C	0.23800	0.10988	-2.47197
C	0.40826	-1.28311	-2.41089
C	0.24688	-1.95425	-1.22640
C	0.22297	2.33471	1.20441
O	-0.36213	2.15046	-1.46278
H	-0.38484	0.87324	3.13526
H	-0.68272	-1.59568	3.27731
H	-0.25345	-2.95344	1.21739
H	0.24701	0.62944	-3.42205
H	0.60515	-1.83135	-3.32404
H	0.28594	-3.03523	-1.17702
H	0.62040	2.51430	2.20063
H	-0.69742	2.89285	1.03783
H	0.96535	2.58455	0.45432
H	-1.28163	2.27504	-0.99095
Cl	-2.81538	2.06324	0.00102

2·Cl, CH_3CN

N	-0.09736	0.86383	1.15160
C	-0.26542	0.20771	2.29321
C	-0.34442	-1.18466	2.35848
C	-0.16315	-1.90109	1.20845
C	0.00466	-1.23383	-0.02708
C	-0.04264	0.18682	-0.05924
C	-0.03059	0.84529	-1.32635
C	0.19191	0.09154	-2.45752
C	0.33372	-1.30700	-2.41147
C	0.20554	-1.96738	-1.21940
C	0.15048	2.32400	1.24873
O	-0.24295	2.17490	-1.46274
H	-0.30379	0.81378	3.18887
H	-0.49122	-1.65504	3.32041
H	-0.14767	-2.98525	1.22028
H	0.21179	0.61458	-3.40662
H	0.49965	-1.85506	-3.33092
H	0.25038	-3.04811	-1.15852
H	0.41541	2.53714	2.28012
H	-0.74857	2.86912	0.97092
H	0.97704	2.58359	0.59513
H	-1.15470	2.37528	-1.11834
Cl	-3.03249	2.39007	-0.41002

2^+, Conf1, gas phase

N	0.64090	1.02814	0.69057
C	0.45044	2.32897	0.49002
C	-0.71850	2.85012	-0.06283
C	-1.71355	1.98050	-0.41393
C	-1.55364	0.58973	-0.21845
C	-0.34073	0.10316	0.35002
C	-0.20128	-1.30307	0.53778
C	-1.23391	-2.13513	0.16687
C	-2.42476	-1.64523	-0.39214
C	-2.58687	-0.30126	-0.58414
C	1.94306	0.62892	1.29024
O	0.94185	-1.78337	1.07521
H	1.26481	2.97739	0.78313
H	-0.80547	3.91897	-0.19760
H	-2.63969	2.34137	-0.84711
H	-1.11363	-3.20334	0.31547
H	-3.20646	-2.34161	-0.66687
H	-3.49523	0.10211	-1.01311
H	2.51707	1.53545	1.45569
H	2.47042	-0.02956	0.60704
H	1.76733	0.11890	2.23232
H	0.90591	-2.74356	1.14795

2^+, Conf1, CH_3CN

N	0.62984	0.96374	0.69908
C	0.49319	2.25949	0.43813
C	-0.64046	2.79380	-0.17304
C	-1.66797	1.94966	-0.48548
C	-1.55759	0.56440	-0.22485
C	-0.36157	0.05308	0.35406
C	-0.26118	-1.35770	0.54705
C	-1.34052	-2.15484	0.24549
C	-2.53407	-1.63649	-0.28494
C	-2.63576	-0.29626	-0.53477
C	1.86641	0.55868	1.41105
O	0.83115	-1.98404	1.07916
H	1.31466	2.89401	0.74109
H	-0.68203	3.85784	-0.35754
H	-2.58272	2.32009	-0.93454
H	-1.23252	-3.21930	0.41779
H	-3.35359	-2.30752	-0.50985
H	-3.52897	0.13729	-0.96811
H	2.35356	1.46387	1.76043
H	2.53307	0.04171	0.72250
H	1.60742	-0.06667	2.25884
H	1.61768	-1.81723	0.54460

nitrophenol·Cl, gas phase

C	-0.50605	0.26810	1.90943
C	-0.61574	-0.97947	1.25568
C	-0.29469	-1.08746	-0.08198
C	0.13788	0.03627	-0.78670
C	0.25367	1.27763	-0.16192
C	-0.06608	1.38933	1.17389
O	-0.79524	0.44217	3.18076
N	0.47378	-0.08454	-2.19304
O	0.36744	-1.17768	-2.72354
O	0.85047	0.91407	-2.78687
H	-0.95455	-1.83474	1.82913
H	-0.37350	-2.03582	-0.59668
H	0.59180	2.13076	-0.73460
H	0.01180	2.33712	1.69171
H	-1.10535	-0.42318	3.63442
Cl	-1.66464	-2.04540	4.39930

nitrophenol·Cl, CH_3CN

C	-0.50127	0.26587	1.88703
C	-0.61078	-0.97627	1.24114
C	-0.28948	-1.08796	-0.09917
C	0.14008	0.04059	-0.79059
C	0.25540	1.28196	-0.16805
C	-0.06577	1.39130	1.16988
O	-0.79729	0.43257	3.17704
N	0.47807	-0.07830	-2.20172
O	0.37272	-1.17006	-2.73255
O	0.85247	0.91960	-2.79253
H	-0.94760	-1.84123	1.80027
H	-0.36999	-2.03984	-0.60726
H	0.59196	2.14343	-0.72945
H	0.01304	2.34180	1.68329
H	-1.09502	-0.41319	3.60222
Cl	-1.71555	-2.08312	4.56942

nitrophenol, Conf1, gas phase

C	-0.50177	0.26901	1.89354
C	-0.61470	-0.96986	1.26010
C	-0.29490	-1.09005	-0.08284
C	0.13371	0.03412	-0.77169
C	0.25154	1.27459	-0.15589
C	-0.06831	1.39095	1.18400
O	-0.79937	0.44688	3.20038
N	0.47340	-0.09140	-2.19637
O	0.36104	-1.18613	-2.70699
O	0.84551	0.90718	-2.77525
H	-0.95203	-1.83706	1.81743
H	-0.37300	-2.03719	-0.59901
H	0.58987	2.12576	-0.73098
H	0.00940	2.33809	1.70167
H	-1.08619	-0.38165	3.59552

nitrophenol, Conf1, CH_3CN

C	-0.50113	0.27001	1.89194
C	-0.61530	-0.97219	1.26044
C	-0.29586	-1.09189	-0.08075
C	0.13401	0.03460	-0.77248
C	0.25260	1.27769	-0.15732
C	-0.06710	1.39393	1.18191
O	-0.79890	0.44231	3.19463
N	0.47146	-0.09019	-2.18783
O	0.36285	-1.18350	-2.71161
O	0.84619	0.90498	-2.78001
H	-0.95307	-1.83594	1.82242
H	-0.37847	-2.04535	-0.58490
H	0.58993	2.13647	-0.72190
H	0.01354	2.34566	1.69226
H	-1.08656	-0.39333	3.58682

nitrocatechol·Cl, gas phase

C	0.40702	0.65474	-1.49353
C	0.03877	1.71521	-0.65581
C	-0.27539	1.52876	0.67790
C	-0.21233	0.23692	1.18204
C	0.15289	-0.84369	0.38570
C	0.46271	-0.66032	-0.95548
O	0.65634	0.95716	-2.76601
O	0.76127	-1.75656	-1.66783
N	-0.53671	0.00457	2.58364
O	-0.84987	0.96402	3.26956
O	-0.48266	-1.13502	3.00997
H	0.00638	2.70068	-1.10374
H	-0.56046	2.35061	1.31873
H	0.19299	-1.84314	0.79598
H	1.08207	0.23199	-3.30768
H	1.16648	-1.58051	-2.55754
Cl	1.98385	-1.17414	-4.33927

nitrocatechol·Cl, CH_3CN

C	0.36275	0.65327	-1.49570
C	0.02654	1.72163	-0.66103
C	-0.26357	1.53128	0.67846
C	-0.20619	0.23699	1.17660
C	0.12831	-0.85039	0.37878
C	0.41143	-0.65655	-0.96467
O	0.58779	0.93675	-2.78952
O	0.66918	-1.75586	-1.70811
N	-0.50414	0.00373	2.58658
O	-0.77705	0.96417	3.28369
O	-0.46783	-1.13944	3.00413
H	-0.00600	2.71296	-1.09690
H	-0.52496	2.36206	1.31886
H	0.16346	-1.85262	0.78518
H	1.06187	0.22957	-3.28283
H	1.15959	-1.56865	-2.53807
Cl	2.17220	-1.17763	-4.29884

nitrocatechol, Conf1, gas phase

C	0.52708	0.68415	-1.41232
C	0.11690	1.74829	-0.62351
C	-0.26532	1.52973	0.69462
C	-0.22182	0.23474	1.18071
C	0.18501	-0.84869	0.41211
C	0.56326	-0.62104	-0.89817
O	0.91994	0.79410	-2.71158
O	0.96384	-1.65279	-1.67230
N	-0.62452	-0.01113	2.57745
O	-0.97646	0.94452	3.23574
O	-0.57921	-1.15251	2.98191
H	0.09578	2.74984	-1.03901
H	-0.58960	2.33786	1.33427
H	0.20737	-1.84855	0.82313
H	0.87507	1.70600	-3.01151
H	1.18980	-1.31820	-2.54830

nitrocatechol, Conf1, CH_3CN

C	0.52729	0.68498	-1.41353
C	0.11600	1.75015	-0.62377
C	-0.26575	1.53098	0.69332
C	-0.22248	0.23479	1.18279
C	0.18579	-0.85124	0.41271
C	0.56319	-0.62165	-0.89555
O	0.91674	0.79673	-2.70322
O	0.96466	-1.65559	-1.66921
N	-0.62231	-0.01060	2.56978
O	-0.97834	0.93875	3.24157
O	-0.58001	-1.15259	2.98638
H	0.09595	2.74976	-1.04362
H	-0.58843	2.34988	1.32103
H	0.21093	-1.85402	0.81783
H	0.87114	1.71512	-3.00237
H	1.19276	-1.32912	-2.55090

nitrocatechol, Conf2, gas phase

C	0.50663	0.67210	-1.42518
C	0.07426	1.73562	-0.64482
C	-0.29555	1.52724	0.67741
C	-0.22259	0.24447	1.19203
C	0.20660	-0.84231	0.43572
C	0.57032	-0.61932	-0.87546
O	0.86358	0.88088	-2.70611
O	1.00964	-1.58323	-1.73668
N	-0.61033	0.00700	2.58968
O	-0.98313	0.95913	3.24015
O	-0.53344	-1.13029	3.00813
H	0.03419	2.72050	-1.09162
H	-0.63549	2.33866	1.30536
H	0.24706	-1.82828	0.88210
H	1.13569	0.04144	-3.09754
H	1.03347	-2.44421	-1.31060

nitrocatechol, Conf2, CH_3CN

C	0.50575	0.67094	-1.42208
C	0.07335	1.73629	-0.64270
C	-0.29610	1.52788	0.67873
C	-0.22209	0.24191	1.19220
C	0.20755	-0.84750	0.43607
C	0.57118	-0.62375	-0.87564
O	0.86185	0.88254	-2.70218
O	1.00799	-1.58295	-1.73160
N	-0.60843	0.00963	2.58287
O	-0.98480	0.96027	3.24199
O	-0.53582	-1.12471	3.01778
H	0.03059	2.72488	-1.08299
H	-0.63440	2.34859	1.29608
H	0.25583	-1.84222	0.86240
H	1.13677	0.04591	-3.10624
H	1.03170	-2.44832	-1.30211

4·Cl, Conf1, gas phase

C	-0.64842	-1.26559	-3.86037
N	-1.93490	-0.67771	-3.50986
N	0.44335	-0.36652	-3.49701
C	-2.59674	-0.97888	-2.38522
N	-3.62886	-0.15213	-2.28104
C	-3.64749	0.69470	-3.37619
C	-2.58494	0.36563	-4.15034
C	1.06009	-0.37647	-2.30646
N	1.92476	0.63056	-2.29165
C	1.86599	1.31003	-3.49584
C	0.93320	0.68525	-4.25452
C	2.77852	0.94970	-1.17260
C	3.61433	-0.03805	-0.68455
C	4.43086	0.25263	0.41246
C	4.37559	1.52365	0.99254
C	3.53100	2.49131	0.46415
C	2.71528	2.22430	-0.62857
O	5.22952	-0.76230	0.80045
C	-4.48633	-0.10597	-1.12213
C	-5.82479	0.21419	-1.26360
C	-3.88551	-0.38200	0.09925
C	-4.68288	-0.35886	1.24175
C	-6.03692	-0.01534	1.13503
C	-6.59279	0.26948	-0.10026
O	-4.22417	-0.63265	2.47507
C	-2.99998	-1.35599	2.63861
C	-1.81834	-0.45922	2.92263
O	-1.50573	0.29694	1.77088
C	-0.26791	0.98371	1.86476
C	0.89996	0.03952	1.91510
C	1.80532	0.03452	2.88820
C	2.91988	-0.95907	2.97802
O	4.11492	-0.27119	3.32744
C	5.28521	-1.05182	3.20410
C	6.05485	-0.64309	1.95868
H	-0.61002	-1.44896	-4.93281
H	-0.53377	-2.19148	-3.29340
H	-2.26298	-1.72776	-1.66198
H	-4.39845	1.45706	-3.49247
H	-2.24645	0.77251	-5.08811
H	0.81242	-1.07836	-1.49599
H	2.50904	2.14879	-3.70217
H	0.60432	0.87396	-5.26264
H	3.66140	-1.02253	-1.13458
H	3.49376	3.46761	0.93094
H	2.03366	2.96709	-1.02399
H	-6.26674	0.38856	-2.23649
H	-2.81792	-0.55438	0.17572
H	-7.64456	0.51708	-0.16801
H	-2.80053	-1.98548	1.76671
H	-3.16586	-1.99966	3.50334
H	-0.97697	-1.10436	3.20253
H	-2.04366	0.21029	3.76345
H	-0.26372	1.64755	2.73990
H	-0.21751	1.60623	0.96698
H	0.93616	-0.70561	1.12029
H	1.74655	0.75385	3.70336
H	3.03505	-1.48719	2.02399
H	2.69883	-1.70542	3.75378
H	5.03679	-2.11732	3.15315
H	5.91264	-0.88885	4.08494
H	6.89219	-1.32097	1.79013
H	6.44961	0.37100	2.04484
H	-6.63236	0.01076	2.03881
H	4.95066	1.75471	1.87607
Cl	-0.52499	-2.45321	-0.55908

4·Cl, Conf1, CH_3CN

C	-0.59593	-1.14625	-3.97448
N	-1.88839	-0.63518	-3.53653
N	0.46441	-0.23784	-3.55500
C	-2.46137	-0.94085	-2.37262
N	-3.57082	-0.21549	-2.25877
C	-3.71504	0.57281	-3.39001
C	-2.65601	0.30930	-4.19146
C	1.13348	-0.33596	-2.40535
N	1.94926	0.71021	-2.31826
C	1.79478	1.50509	-3.44261
C	0.86012	0.90821	-4.21975
C	2.82580	0.97939	-1.21230
C	3.61362	-0.04712	-0.71938
C	4.44758	0.20473	0.37449
C	4.47158	1.47879	0.94757
C	3.67549	2.48818	0.41514
C	2.83790	2.25787	-0.66892
O	5.19771	-0.85197	0.76935
C	-4.44397	-0.22521	-1.11843
C	-5.80823	-0.06968	-1.30700
C	-3.86796	-0.36666	0.13918
C	-4.70401	-0.36853	1.25395
C	-6.08232	-0.19324	1.09383
C	-6.62071	-0.04227	-0.17501
O	-4.25183	-0.49724	2.52367
C	-3.02154	-1.18875	2.77258
C	-1.86763	-0.26134	3.06264
O	-1.50144	0.44466	1.89204
C	-0.27301	1.15543	2.03208
C	0.90400	0.22590	1.96607
C	1.73829	0.00346	2.97839
C	2.84910	-0.99592	2.92509
O	4.05619	-0.36961	3.34611
C	5.20261	-1.18678	3.17729
C	5.99771	-0.77704	1.95198
H	-0.59225	-1.21242	-5.05926
H	-0.42853	-2.11735	-3.51212
H	-2.06522	-1.65236	-1.65485
H	-4.54463	1.24960	-3.50900
H	-2.37507	0.70148	-5.15509
H	0.99884	-1.12287	-1.66856
H	2.37706	2.40001	-3.58593
H	0.45208	1.17664	-5.18042
H	3.60460	-1.03240	-1.17133
H	3.69825	3.47102	0.87069
H	2.19928	3.03562	-1.06901
H	-6.22745	0.01743	-2.30166
H	-2.79329	-0.41790	0.25757
H	-7.69084	0.08099	-0.29059
H	-2.78768	-1.85712	1.93968
H	-3.20296	-1.79474	3.66198
H	-1.03510	-0.87856	3.42228
H	-2.14110	0.44590	3.85655
H	-0.26852	1.71978	2.97267
H	-0.24719	1.86476	1.20148
H	1.03350	-0.31774	1.03021
H	1.60934	0.53719	3.91925
H	2.94691	-1.39767	1.91003
H	2.62890	-1.83487	3.60042
H	4.91076	-2.23966	3.09806
H	5.84168	-1.07504	4.05795
H	6.81363	-1.48517	1.79908
H	6.43069	0.21770	2.06525
H	-6.71352	-0.18509	1.97447
H	5.07967	1.69240	1.81404
Cl	-0.21877	-3.01180	-0.75327

4·Cl, Conf2, gas phase

C	-0.44561	-0.82365	-3.66005
N	-1.62202	-0.08322	-3.22198
N	0.76827	-0.05596	-3.41056
C	-2.48456	-0.54554	-2.31162
N	-3.37255	0.40661	-2.05981
C	-3.08097	1.51626	-2.83454
C	-1.98506	1.20882	-3.56935
C	1.39034	0.07258	-2.22639
N	2.45397	0.84887	-2.41586
C	2.51900	1.22760	-3.74536
C	1.45854	0.66441	-4.36913
C	3.44251	1.20955	-1.42709
C	3.90549	0.22393	-0.56375
C	4.93344	0.56312	0.31854
C	5.42859	1.87403	0.33650
C	4.91688	2.83408	-0.51523
C	3.91110	2.51238	-1.42440
O	5.55034	-0.28919	1.15511
C	-4.37532	0.29121	-1.03076
C	-5.65751	0.75398	-1.26525
C	-3.96817	-0.30166	0.15799
C	-4.92428	-0.47349	1.15836
C	-6.22949	-0.00422	0.95704
C	-6.58384	0.60689	-0.23287
O	-4.68527	-1.06779	2.33942
C	-3.45761	-1.76196	2.57016
C	-2.44143	-0.88960	3.26599
O	-2.00312	0.11528	2.37511
C	-1.12412	1.04352	2.97412
C	0.25127	0.49280	3.25250
C	0.76846	-0.57690	2.65714
C	2.08338	-1.15674	3.06630
O	2.97713	-1.21087	1.96345
C	4.16061	-1.89206	2.30248
C	5.18655	-1.66470	1.21892
H	-0.50062	-1.01648	-4.73053
H	-0.40669	-1.74739	-3.07903
H	-2.42054	-1.50842	-1.82483
H	-3.66512	2.41831	-2.77227
H	-1.43196	1.79200	-4.28596

H	1.04408	-0.40467	-1.30452
H	3.32863	1.82904	-4.12107
H	1.15568	0.68188	-5.40275
H	3.46715	-0.76454	-0.57770
H	5.30395	3.84448	-0.47963
H	3.49581	3.25818	-2.09027
H	-5.93615	1.18547	-2.21845
H	-2.92731	-0.56523	0.31256
H	-7.59966	0.95419	-0.37305
H	-3.05282	-2.16889	1.63940
H	-3.72148	-2.59218	3.22600
H	-1.60546	-1.51937	3.59150
H	-2.90047	-0.43110	4.15213
H	-1.56219	1.42036	3.90874
H	-1.05984	1.89124	2.28625
H	0.82470	1.02028	4.01293
H	0.21531	-1.10463	1.88213
H	1.92824	-2.17760	3.44538
H	2.53329	-0.56308	3.87317
H	3.97647	-2.96984	2.41329
H	4.56166	-1.51091	3.25127
H	4.83870	-2.02606	0.24895
H	6.10550	-2.19537	1.46959
H	-6.94874	-0.13858	1.75504
H	6.22475	2.10499	1.03273
Cl	-0.44231	-1.92607	-0.56163

4·Cl, Conf2, CH_3CN

C	-0.38205	-0.71168	-3.84477
N	-1.62045	-0.10535	-3.37270
N	0.76105	0.11388	-3.48032
C	-2.28522	-0.49671	-2.28670
N	-3.34918	0.29145	-2.15094
C	-3.36415	1.21429	-3.18537
C	-2.27871	0.96295	-3.95386
C	1.45413	0.00206	-2.34627
N	2.39214	0.94580	-2.34775
C	2.29325	1.68480	-3.51598
C	1.26705	1.16167	-4.22657
C	3.36355	1.16156	-1.31135
C	3.96695	0.05556	-0.72688
C	4.91345	0.27371	0.27476
C	5.24711	1.57954	0.64453
C	4.62875	2.66094	0.03462
C	3.66606	2.46690	-0.95127
O	5.61706	-0.71254	0.88366
C	-4.33197	0.17444	-1.11023
C	-5.65930	0.43472	-1.41190
C	-3.90466	-0.19772	0.16070
C	-4.86429	-0.34248	1.16171
C	-6.20885	-0.06794	0.88710
C	-6.59422	0.32254	-0.38482
O	-4.58383	-0.71346	2.43168
C	-3.37644	-1.41971	2.73725
C	-2.33462	-0.52558	3.35925
O	-1.79325	0.33697	2.37394
C	-0.87332	1.27214	2.90165
C	0.48418	0.69856	3.20274
C	0.90681	-0.50365	2.82437
C	2.24497	-1.05885	3.19385
O	2.99703	-1.29647	2.01210
C	4.15766	-2.06128	2.26579
C	5.05141	-2.01556	1.05158
H	-0.41807	-0.78639	-4.92859
H	-0.27611	-1.68791	-3.37518
H	-1.98920	-1.31667	-1.64239
H	-4.13495	1.96151	-3.26885
H	-1.91044	1.43953	-4.84757
H	1.26287	-0.73072	-1.57009
H	2.97491	2.48904	-3.73643
H	0.86131	1.41813	-5.19129
H	3.70668	-0.93893	-1.06326
H	4.88807	3.66800	0.33842
H	3.15657	3.30139	-1.41656
H	-5.96014	0.70154	-2.41707
H	-2.85156	-0.32457	0.37573
H	-7.63892	0.52252	-0.59041
H	-2.98913	-1.92731	1.84974
H	-3.66145	-2.17703	3.46949
H	-1.55626	-1.16016	3.79794
H	-2.79142	0.06564	4.16325
H	-1.28411	1.72973	3.81168
H	-0.77604	2.06979	2.15893
H	1.14225	1.34493	3.78180
H	0.25605	-1.15172	2.24111
H	2.11629	-2.00695	3.73515
H	2.78746	-0.36450	3.84823
H	3.89278	-3.10525	2.48157
H	4.70024	-1.65649	3.13043
H	4.51907	-2.34257	0.15688
H	5.90240	-2.67945	1.20424
H	-6.93461	-0.17493	1.68446
H	5.99344	1.72463	1.41651
Cl	-0.10860	-2.75197	-0.92694

4^{2+}, Conf1, gas phase

C	-0.37256	-0.46642	-4.10149
N	-1.17992	0.34414	-3.20189
N	1.02944	-0.06514	-4.03152
C	-1.95413	-0.13458	-2.21459
N	-2.56342	0.88712	-1.62923
C	-2.18114	2.05812	-2.25748
C	-1.32018	1.72113	-3.24918
C	1.72905	0.16939	-2.90928
N	2.97985	0.44907	-3.25102
C	3.09911	0.38673	-4.62485
C	1.87610	0.06793	-5.11878
C	4.01667	0.79131	-2.30421
C	3.98686	0.13421	-1.08079
C	4.90145	0.52247	-0.10603
C	5.84717	1.51499	-0.40185
C	5.86004	2.12562	-1.64217
C	4.92603	1.78273	-2.62203
O	4.95201	0.00140	1.12932
C	-3.47242	0.78849	-0.50791
C	-4.61218	1.58178	-0.50438
C	-3.15680	-0.09005	0.51204
C	-4.03031	-0.19369	1.60118
C	-5.17763	0.60597	1.64173
C	-5.45535	1.47777	0.59513
O	-3.67519	-1.07349	2.54426
C	-4.36924	-1.06098	3.79770
C	-3.61780	-1.98846	4.72696
O	-2.30546	-1.53191	4.95392
C	-1.28629	-2.06882	4.13060
C	-0.58724	-0.97883	3.37100
C	-0.13522	-1.09737	2.12603
C	0.62583	-0.02038	1.40874
O	1.89728	-0.45537	0.93761
C	2.78639	-0.77637	2.00332
C	4.16342	-1.13230	1.48471
H	-0.70672	-0.32868	-5.12962
H	-0.48761	-1.51305	-3.81845
H	-2.08905	-1.17444	-1.95763
H	-2.54432	3.01867	-1.93063
H	-0.79492	2.33041	-3.96692
H	1.35316	0.16257	-1.89576
H	4.03964	0.55655	-5.12236
H	1.54405	-0.09126	-6.13194
H	3.25699	-0.63570	-0.88000
H	6.59391	2.89310	-1.85264
H	4.89963	2.29946	-3.57310
H	-4.85379	2.23281	-1.33507
H	-2.24048	-0.66809	0.53205
H	-6.35569	2.07803	0.63180
H	-5.39952	-1.40526	3.66103
H	-4.36366	-0.04374	4.20027
H	-3.61939	-3.00719	4.32469
H	-4.13191	-2.00364	5.69026
H	-1.68470	-2.81777	3.43940
H	-0.55904	-2.56285	4.78556
H	-0.42328	-0.05775	3.92817
H	-0.28925	-2.02819	1.57889
H	0.74396	0.85637	2.05703
H	0.08615	0.30494	0.50884
H	2.40013	-1.63414	2.56452
H	2.86763	0.07535	2.68977
H	4.11188	-1.84488	0.65607
H	4.71902	-1.60154	2.29636
H	-5.85941	0.54873	2.47915
H	6.56284	1.78452	0.36477

4^{2+}, Conf1, CH_3CN

C	-0.40818	-0.54380	-4.15921
N	-1.33018	0.24165	-3.35285
N	0.94759	-0.02009	-4.02856
C	-2.04790	-0.23574	-2.33752
N	-2.78379	0.75880	-1.84840
C	-2.52729	1.90969	-2.57800
C	-1.61615	1.58403	-3.52387
C	1.63309	0.08889	-2.89059
N	2.84213	0.56311	-3.17945
C	2.93289	0.76204	-4.54746
C	1.74147	0.39896	-5.07878
C	3.87866	0.83606	-2.21991
C	3.98790	-0.00085	-1.11425
C	4.97553	0.27583	-0.16959
C	5.83761	1.36141	-0.36404
C	5.70216	2.17129	-1.47943
C	4.71038	1.92576	-2.42665
O	5.20071	-0.45403	0.94640
C	-3.68255	0.65975	-0.73193
C	-4.88211	1.36452	-0.76805
C	-3.31634	-0.12151	0.34961
C	-4.18347	-0.21081	1.44204
C	-5.38786	0.49505	1.44035
C	-5.72091	1.27376	0.33405
O	-3.76212	-0.99951	2.45406
C	-4.42031	-0.89595	3.71665
C	-3.59453	-1.66686	4.72130
O	-2.29466	-1.11649	4.83126
C	-1.29444	-1.82504	4.10149
C	-0.19483	-0.87303	3.75015
C	0.24418	-0.69440	2.50731
C	1.31754	0.27957	2.11815
O	2.34807	-0.32567	1.35067
C	3.19003	-1.16777	2.11350
C	4.37641	-1.57422	1.27320
H	-0.68600	-0.47508	-5.20772
H	-0.44550	-1.57449	-3.81393
H	-2.04071	-1.25644	-1.98584
H	-3.00322	2.84709	-2.34366
H	-1.13894	2.17338	-4.29018

H	1.26358	-0.14383	-1.90319
H	3.83343	1.12634	-5.01207
H	1.38636	0.38592	-6.09591
H	3.30527	-0.82897	-0.99380
H	6.36896	3.01497	-1.61172
H	4.57944	2.57196	-3.28510
H	-5.15210	1.95660	-1.63347
H	-2.36713	-0.64325	0.38290
H	-6.66085	1.81269	0.33194
H	-5.43101	-1.31306	3.65890
H	-4.47908	0.15732	4.00951
H	-3.54755	-2.72602	4.44663
H	-4.08380	-1.59104	5.69587
H	-1.71578	-2.25290	3.18836
H	-0.91171	-2.64344	4.72629
H	0.24521	-0.30855	4.57114
H	-0.19730	-1.26584	1.69079
H	1.74007	0.75994	3.00984
H	0.89516	1.05732	1.47626
H	2.66230	-2.07447	2.43620
H	3.53928	-0.63537	3.00806
H	4.07260	-2.11175	0.37227
H	5.01131	-2.23663	1.86254
H	-6.06627	0.44080	2.28151
H	6.60576	1.55188	0.37601

4^{2+}, Conf2, gas phase

C	-0.65838	-0.91549	-3.92518
N	-1.64494	-0.13745	-3.18640
N	0.65679	-0.28932	-3.87702
C	-2.49213	-0.64327	-2.27477
N	-3.31910	0.31827	-1.89214
C	-3.00658	1.47753	-2.57672
C	-1.96440	1.19374	-3.39696
C	1.37830	-0.04867	-2.76962
N	2.54039	0.47382	-3.13565
C	2.57780	0.57549	-4.51279
C	1.39696	0.10035	-4.98097
C	3.59270	0.87030	-2.22626
C	3.88051	0.03336	-1.16320
C	4.85963	0.42843	-0.24690
C	5.54758	1.62976	-0.45185
C	5.23577	2.43662	-1.53872
C	4.24244	2.07762	-2.44316
O	5.09633	-0.42502	0.75497
C	-4.39635	0.15737	-0.93731
C	-5.63133	0.69365	-1.25297
C	-4.12671	-0.53883	0.23658
C	-5.18266	-0.72953	1.13102
C	-6.44156	-0.18108	0.84608
C	-6.65748	0.52334	-0.32307
O	-5.08737	-1.39709	2.29008
C	-4.00644	-2.29172	2.54614
C	-2.92703	-1.64548	3.38122
O	-2.26446	-0.66380	2.60916
C	-1.39850	0.16911	3.37486
C	-0.06283	-0.46519	3.63313
C	1.08861	0.18215	3.49471
C	2.42461	-0.38428	3.85664
O	3.34493	-0.02983	2.84141
C	4.64451	-0.51845	3.08127
C	5.54492	0.07070	2.02321
H	-0.94895	-0.98676	-4.97309
H	-0.61814	-1.91574	-3.49399
H	-2.52572	-1.66635	-1.93235
H	-3.54413	2.39543	-2.40377
H	-1.42189	1.81512	-4.09077
H	1.06686	-0.22036	-1.75029
H	3.44586	0.95131	-5.02901
H	1.03341	-0.01754	-5.98900
H	3.39465	-0.92453	-1.02155
H	5.77500	3.36433	-1.68288
H	3.97546	2.72558	-3.26852
H	-5.80672	1.19742	-2.19541
H	-3.12002	-0.83802	0.49957
H	-7.63971	0.92754	-0.53213
H	-3.60582	-2.68525	1.60745
H	-4.44451	-3.11822	3.10650
H	-2.23196	-2.42532	3.71771
H	-3.38645	-1.18564	4.26436
H	-1.89343	0.42043	4.32154
H	-1.27249	1.09527	2.81126
H	-0.06404	-1.48959	4.00156
H	1.10043	1.21271	3.14375
H	2.36694	-1.47517	3.96603
H	2.76171	0.03335	4.81632
H	4.66260	-1.61446	3.03155
H	5.00660	-0.20791	4.07049
H	6.58411	-0.22713	2.17387
H	5.46060	1.15871	2.05293
H	-7.23591	-0.33161	1.56641
H	6.34089	1.92489	0.22235

4^{2+}, Conf2, CH_3CN

C	-0.73217	-0.85890	-4.19647
N	-1.64251	-0.07762	-3.37226
N	0.61914	-0.31545	-4.10963
C	-2.41875	-0.58314	-2.41449
N	-3.16867	0.40124	-1.92674
C	-2.85942	1.57537	-2.59509
C	-1.90544	1.27369	-3.50655
C	1.31157	-0.12170	-2.98780
N	2.51161	0.34884	-3.32049
C	2.58950	0.45309	-4.69910
C	1.39892	0.03932	-5.19315
C	3.53877	0.72626	-2.38949
C	3.65936	0.01551	-1.20805
C	4.61266	0.42137	-0.27160
C	5.45863	1.49547	-0.55374
C	5.32019	2.17627	-1.75996
C	4.35361	1.81333	-2.68885
O	4.65481	-0.29767	0.86986
C	-4.19524	0.24518	-0.93109
C	-5.39413	0.91392	-1.11729
C	-3.94973	-0.58713	0.15739
C	-4.98088	-0.78804	1.07650
C	-6.19771	-0.11352	0.91512
C	-6.39287	0.73278	-0.16278
O	-4.91352	-1.60565	2.15010
C	-3.79254	-2.46623	2.35877
C	-2.83638	-1.87696	3.36553
O	-2.28389	-0.68516	2.84273
C	-1.53783	0.05415	3.80203
C	-0.15418	-0.49518	3.99800
C	0.93800	0.26293	3.98234
C	2.32342	-0.25011	4.21497
O	3.13654	0.21083	3.14965
C	4.46842	-0.24881	3.22849
C	5.21228	0.30468	2.04087
H	-1.04034	-0.80286	-5.23759
H	-0.74837	-1.88730	-3.84318
H	-2.45072	-1.61764	-2.10810
H	-3.33842	2.50873	-2.35119
H	-1.38286	1.88716	-4.22250
H	0.95018	-0.29007	-1.98542
H	3.48148	0.79634	-5.19529
H	1.03647	-0.04865	-6.20398
H	3.03012	-0.83841	-0.98748
H	5.97342	3.01377	-1.97329
H	4.22727	2.36908	-3.60917
H	-5.55219	1.54015	-1.98619
H	-2.97281	-1.03065	0.29129
H	-7.34143	1.24318	-0.27834
H	-3.29725	-2.70191	1.41559
H	-4.20202	-3.39135	2.76742
H	-2.05971	-2.62103	3.58352
H	-3.37699	-1.66017	4.29589
H	-2.08505	0.06141	4.75443
H	-1.48265	1.08125	3.43601
H	-0.06701	-1.56518	4.18091
H	0.85356	1.33332	3.79820
H	2.32748	-1.34696	4.25661
H	2.72085	0.12858	5.16801
H	4.49758	-1.34625	3.22163
H	4.95025	0.10543	4.14933
H	6.27916	0.07482	2.10881
H	5.07674	1.38863	2.00394
H	-6.97871	-0.27454	1.64867
H	6.22021	1.79774	0.15344

4^{2+}, Conf3, gas phase

C	-0.31481	-1.61571	-2.73162
N	-1.61503	-0.96148	-2.70726
N	0.78102	-0.66182	-2.83815
C	-2.29367	-0.64530	-1.59391
N	-3.42503	-0.05255	-1.95682
C	-3.48055	0.02667	-3.33444
C	-2.34475	-0.54296	-3.80911
C	1.53174	-0.21568	-1.81690
N	2.42287	0.63886	-2.30092
C	2.24450	0.75630	-3.66580
C	1.21463	-0.05687	-4.00542
C	3.45420	1.29218	-1.52541
C	4.13103	0.51520	-0.59462
C	5.11580	1.12926	0.17856
C	5.39716	2.48866	-0.01758
C	4.70242	3.22511	-0.95975
C	3.70392	2.63592	-1.73664
O	5.85284	0.50434	1.10978
C	-4.40358	0.38570	-0.99188
C	-5.01894	1.62391	-1.10653
C	-4.60108	-0.45112	0.09036
C	-5.35151	0.01069	1.16216
C	-6.00518	1.23714	1.07280
C	-5.85442	2.02310	-0.06701
O	-5.46002	-0.75800	2.27962
C	-4.30414	-0.79821	3.12196
C	-3.13243	-1.61636	2.58178
O	-2.29426	-0.92324	1.64831
C	-1.30410	-0.10350	2.26522
C	-0.03916	-0.86450	2.53776
C	1.18159	-0.36959	2.34988
C	2.43117	-1.04071	2.82718
O	3.42890	-0.94939	1.82683
C	4.71923	-1.27325	2.31972
C	5.76614	-0.90649	1.29302
H	-0.27699	-2.29018	-3.58640
H	-0.19283	-2.19192	-1.81536
H	-2.00635	-0.84009	-0.56265
H	-4.33069	0.44660	-3.84677
H	-2.01653	-0.71575	-4.82097

H	1.44053	-0.50112	-0.77630
H	2.88757	1.37770	-4.26716
H	0.78320	-0.27927	-4.96755
H	3.88706	-0.52901	-0.46761
H	4.93245	4.27444	-1.09368
H	3.13524	3.21374	-2.45452
H	-4.83791	2.26995	-1.95710
H	-4.16473	-1.43940	0.12441
H	-6.36402	2.97605	-0.13140
H	-4.65755	-1.26949	4.03900
H	-3.99077	0.22518	3.35834
H	-3.51033	-2.50735	2.07666
H	-2.52824	-1.95327	3.43118
H	-1.69708	0.31364	3.19982
H	-1.11246	0.74138	1.59742
H	-0.15595	-1.84876	2.98927
H	1.31511	0.62772	1.92908
H	2.23806	-2.08812	3.09131
H	2.78015	-0.52596	3.73314
H	4.79084	-2.34578	2.54149
H	4.91570	-0.71275	3.24121
H	5.60241	-1.41280	0.33810
H	6.74506	-1.20525	1.66782
H	-6.62374	1.56346	1.90007
H	6.17631	2.93960	0.58421

4^{2+}, Conf3, CH_3CN

C	-0.25493	-1.54823	-3.53951
N	-1.44394	-0.79315	-3.17279
N	0.91970	-0.68608	-3.51860
C	-1.97790	-0.76965	-1.95279
N	-2.99659	0.08448	-1.96514
C	-3.11544	0.62941	-3.23315
C	-2.13844	0.07764	-3.99161
C	1.58779	-0.32364	-2.42296
N	2.56070	0.50554	-2.78891
C	2.51425	0.67717	-4.16334
C	1.48051	-0.06804	-4.61960
C	3.50027	1.14444	-1.90703
C	3.98525	0.43205	-0.81340
C	4.90964	1.06026	0.02114
C	5.31403	2.37394	-0.25032
C	4.80122	3.05403	-1.34076
C	3.87941	2.44626	-2.19063
O	5.50070	0.49023	1.09355
C	-3.79691	0.40897	-0.81691
C	-4.07631	1.74372	-0.54643
C	-4.20668	-0.61969	0.01624
C	-4.89472	-0.29593	1.18122
C	-5.19358	1.03241	1.47738
C	-4.78896	2.04218	0.60904
O	-5.30479	-1.31387	1.99519
C	-4.71256	-1.33556	3.30184
C	-3.41509	-2.12512	3.28070
O	-2.50814	-1.65478	2.29906
C	-1.84330	-0.43682	2.61591
C	-0.44675	-0.71233	3.08614
C	0.64151	-0.13049	2.58929
C	2.01229	-0.35627	3.14190
O	2.93118	-0.56795	2.07882
C	4.20660	-0.92198	2.57608
C	5.23253	-0.86079	1.47340
H	-0.37531	-1.93348	-4.54805
H	-0.12166	-2.35630	-2.82553
H	-1.63122	-1.33313	-1.09960
H	-3.89128	1.33739	-3.47255
H	-1.87937	0.20882	-5.02945
H	1.36389	-0.63599	-1.41398
H	3.23060	1.29001	-4.68345
H	1.10319	-0.23258	-5.61546
H	3.64585	-0.57847	-0.63208
H	5.11765	4.07167	-1.53529
H	3.45983	2.97480	-3.03719
H	-3.72661	2.52546	-1.20986
H	-3.98005	-1.65546	-0.20364
H	-5.02288	3.07433	0.84017
H	-5.42513	-1.82992	3.96383
H	-4.56486	-0.31284	3.65825
H	-3.62823	-3.16263	3.01645
H	-2.96645	-2.10704	4.28268
H	-2.39757	0.11159	3.38672
H	-1.83073	0.18288	1.71330
H	-0.35224	-1.42981	3.90110
H	0.55688	0.58769	1.77427
H	2.00834	-1.22054	3.81849
H	2.33688	0.52089	3.72020
H	4.18715	-1.94003	2.98765
H	4.50356	-0.23372	3.37824
H	4.94475	-1.46715	0.61352
H	6.17791	-1.24640	1.85790
H	-5.74317	1.26906	2.38144
H	6.03774	2.83803	0.40913

4^{2+}, Conf4, gas phase

C	-0.42798	-1.03171	-3.22289
N	-1.26218	-0.04905	-2.54887
N	0.94421	-0.56059	-3.37564
C	-1.86902	-0.24141	-1.36647
N	-2.62995	0.81759	-1.11844
C	-2.50167	1.72609	-2.15268
C	-1.64548	1.18469	-3.05382
C	1.74740	-0.17701	-2.37219
N	2.94678	0.08538	-2.87793
C	2.92194	-0.13142	-4.24102
C	1.66553	-0.53592	-4.55740
C	4.06057	0.52474	-2.07141
C	4.10626	0.01622	-0.78232
C	5.03375	0.54176	0.10750
C	5.97285	1.47352	-0.35270
C	5.93517	1.91334	-1.66531
C	4.95112	1.46743	-2.55058
O	5.08998	0.20457	1.40932
C	-3.48203	0.90394	0.04175
C	-3.54719	2.07024	0.79454
C	-4.15372	-0.25053	0.39508
C	-4.83861	-0.28129	1.60290
C	-4.94465	0.87454	2.37197
C	-4.31447	2.04648	1.95492
O	-5.40103	-1.45648	1.99516
C	-4.55810	-2.29180	2.79767
C	-3.43353	-2.97858	2.02874
O	-2.41120	-2.12812	1.50802
C	-1.75606	-1.34466	2.49482
C	-0.50083	-0.76568	1.91692
C	-0.28907	0.54591	1.84295
C	0.97736	1.20259	1.36688
O	2.04294	0.30501	1.13662
C	2.80988	0.02010	2.30921
C	4.11666	-0.67165	1.96932
H	-0.82402	-1.22876	-4.21861
H	-0.44728	-1.95198	-2.63895
H	-1.77175	-1.09544	-0.70327
H	-3.05400	2.65153	-2.16780
H	-1.29617	1.55233	-4.00506
H	1.48023	-0.07957	-1.32690
H	3.79783	-0.00130	-4.85491
H	1.23521	-0.82553	-5.50237
H	3.40275	-0.73793	-0.47028
H	6.66167	2.64120	-2.00346
H	4.87390	1.87376	-3.55115
H	-3.00751	2.96250	0.49941
H	-4.13000	-1.14162	-0.21822
H	-4.40293	2.94454	2.55323
H	-5.21667	-3.06984	3.18383
H	-4.18053	-1.71858	3.65119
H	-3.84967	-3.50443	1.16803
H	-2.98048	-3.72036	2.69905
H	-1.51360	-1.97601	3.36063
H	-2.40701	-0.53072	2.83757
H	0.27305	-1.46585	1.60826
H	-1.07002	1.23033	2.17340
H	1.27866	1.97583	2.08435
H	0.79125	1.72748	0.42049
H	2.23704	-0.62481	2.98554
H	3.03796	0.95630	2.83045
H	3.96675	-1.55121	1.33644
H	4.56493	-1.01221	2.90246
H	-5.52029	0.84694	3.28978
H	6.71526	1.84516	0.34256

4^{2+}, Conf4, CH_3CN

C	-0.42775	-0.80698	-4.01009
N	-1.26306	0.04907	-3.19147
N	0.97542	-0.39881	-3.89817
C	-1.77700	-0.29936	-2.01132
N	-2.45505	0.73849	-1.53360
C	-2.37190	1.78706	-2.43650
C	-1.62390	1.35417	-3.47802
C	1.59406	-0.01503	-2.78356
N	2.87578	0.19676	-3.07383
C	3.08313	-0.06424	-4.41621
C	1.88763	-0.43717	-4.93382
C	3.86296	0.65951	-2.13730
C	3.79893	0.18183	-0.83244
C	4.72110	0.66551	0.09359
C	5.69478	1.58687	-0.31168
C	5.73590	2.03035	-1.62320
C	4.81046	1.57695	-2.56166
O	4.76849	0.29947	1.39400
C	-3.13151	0.76094	-0.26659
C	-3.07570	1.91391	0.50672
C	-3.78176	-0.38756	0.15771
C	-4.38444	-0.39049	1.41305
C	-4.35515	0.75695	2.20707
C	-3.70511	1.89726	1.74665
O	-5.05973	-1.51596	1.77823
C	-4.74858	-2.08372	3.05669
C	-3.57164	-3.03580	2.93104
O	-2.42352	-2.41668	2.38434
C	-1.74122	-1.56435	3.29479
C	-0.58884	-0.93331	2.57847
C	-0.41610	0.38348	2.50806
C	0.72613	1.08360	1.82676
O	1.77937	0.23613	1.41526
C	2.62830	-0.17648	2.47356
C	3.91631	-0.72669	1.91000
H	-0.71642	-0.70901	-5.05382
H	-0.54291	-1.83291	-3.66801
H	-1.64552	-1.25507	-1.52686
H	-2.86775	2.72653	-2.25923
H	-1.32322	1.83726	-4.39318

H	1.13944	0.12864	-1.81530
H	4.05515	0.03005	-4.87003
H	1.60110	-0.73026	-5.93025
H	3.03486	-0.52837	-0.55141
H	6.49048	2.74799	-1.92180
H	4.81658	1.94160	-3.58138
H	-2.54438	2.79108	0.15822
H	-3.82549	-1.27666	-0.45973
H	-3.68314	2.78560	2.36651
H	-5.63130	-2.64203	3.37061
H	-4.56474	-1.29691	3.79077
H	-3.83554	-3.84349	2.24552
H	-3.35392	-3.46909	3.91680
H	-1.38773	-2.16393	4.14576
H	-2.40715	-0.78432	3.68159
H	0.13079	-1.60870	2.12018
H	-1.14858	1.04533	2.96854
H	1.11456	1.87125	2.48615
H	0.35484	1.58050	0.92388
H	2.15445	-0.95775	3.07876
H	2.85418	0.67549	3.12709
H	3.73147	-1.49604	1.15680
H	4.48259	-1.17831	2.72533
H	-4.84929	0.76450	3.17126
H	6.40999	1.94134	0.42098

4^{2+}, Conf5, gas phase

C	-0.40083	-0.97714	-3.26454
N	-1.59122	-0.21380	-2.90320
N	0.80702	-0.17357	-3.16697
C	-2.48021	-0.57743	-1.96608
N	-3.46132	0.31375	-1.94890
C	-3.20653	1.27800	-2.90509
C	-2.04023	0.94551	-3.51191
C	1.52422	0.05736	-2.05256
N	2.54664	0.83725	-2.37337
C	2.49319	1.12530	-3.72386
C	1.40305	0.49478	-4.22408
C	3.59606	1.27264	-1.47567
C	4.16629	0.31833	-0.64152
C	5.20814	0.72348	0.19459
C	5.62387	2.06313	0.17789
C	5.01879	2.98272	-0.65791
C	3.98481	2.59937	-1.51274
O	5.89174	-0.08559	1.01609
C	-4.58561	0.28627	-1.03929
C	-5.82926	0.69258	-1.48817
C	-4.33730	-0.14222	0.25830
C	-5.40616	-0.17413	1.15192
C	-6.67248	0.25616	0.73686
C	-6.87505	0.68277	-0.56420
O	-5.28635	-0.56327	2.43385
C	-4.28311	-1.50555	2.81394
C	-3.04390	-0.86775	3.40205
O	-2.24033	-0.30967	2.37376
C	-1.05656	0.31510	2.85406
C	0.08841	-0.64925	2.96051
C	1.33272	-0.36642	2.58674
C	2.50563	-1.24423	2.88673
O	3.39097	-1.26165	1.77870
C	4.63989	-1.84356	2.10639
C	5.65339	-1.49062	1.04323
H	-0.48781	-1.32774	-4.29280
H	-0.32728	-1.83584	-2.59852
H	-2.42506	-1.45662	-1.34279
H	-3.86466	2.11866	-3.05005
H	-1.49514	1.43613	-4.30125
H	1.31571	-0.32009	-1.06083
H	3.25386	1.71957	-4.20303
H	1.02674	0.42852	-5.23234
H	3.80997	-0.70165	-0.64499
H	5.35289	4.01242	-0.65235
H	3.49518	3.31553	-2.16085
H	-5.99801	0.98143	-2.51808
H	-3.33596	-0.35642	0.60962
H	-7.86347	0.99420	-0.87717
H	-4.02821	-2.14814	1.96530
H	-4.75298	-2.11899	3.58328
H	-2.48824	-1.64359	3.94384
H	-3.33797	-0.08900	4.11498
H	-1.25778	0.77092	3.83153
H	-0.81173	1.12466	2.16238
H	-0.12347	-1.60449	3.43856
H	1.56886	0.59732	2.13533
H	2.17921	-2.26108	3.13913
H	3.03635	-0.83756	3.75865
H	4.55553	-2.93498	2.18602
H	4.99221	-1.45197	3.06789
H	5.36408	-1.85671	0.05525
H	6.61221	-1.94087	1.30035
H	-7.48246	0.23845	1.45525
H	6.43874	2.34924	0.83116

4^{2+}, Conf5, CH_3CN

C	-0.43037	-0.91034	-3.58046
N	-1.61948	-0.18442	-3.15015
N	0.76433	-0.10298	-3.37799
C	-2.40691	-0.54793	-2.14020
N	-3.39953	0.33387	-2.04928
C	-3.23889	1.29284	-3.03714
C	-2.12492	0.96356	-3.73148
C	1.48805	-0.05252	-2.25799
N	2.48317	0.80783	-2.45135
C	2.39238	1.32757	-3.73223
C	1.31390	0.75435	-4.31393
C	3.50998	1.14685	-1.50233
C	4.11597	0.12342	-0.78318
C	5.13145	0.46102	0.11297
C	5.51252	1.79953	0.25771
C	4.88440	2.79319	-0.47587
C	3.86416	2.48055	-1.37028
O	5.85385	-0.42833	0.83365
C	-4.46773	0.28320	-1.08868
C	-5.72722	0.72559	-1.46234
C	-4.18735	-0.20319	0.18373
C	-5.22646	-0.26442	1.11117
C	-6.50162	0.19443	0.76553
C	-6.74085	0.68721	-0.50730
O	-5.07661	-0.72021	2.37701
C	-4.03698	-1.65469	2.68693
C	-2.86373	-1.00794	3.38009
O	-2.14660	-0.20760	2.45961
C	-1.06786	0.50933	3.04880
C	0.12984	-0.35878	3.30290
C	1.35144	-0.07011	2.86321
C	2.56342	-0.87808	3.19950
O	3.31282	-1.10018	2.01557
C	4.49887	-1.82524	2.26755
C	5.38804	-1.76149	1.05029
H	-0.51090	-1.13190	-4.64146
H	-0.35316	-1.82412	-2.99596
H	-2.27031	-1.41992	-1.51935
H	-3.91882	2.12102	-3.14424
H	-1.64041	1.43961	-4.56845
H	1.29724	-0.60848	-1.35271
H	3.11538	2.03207	-4.10769
H	0.89398	0.85787	-5.30108
H	3.80410	-0.89875	-0.94467
H	5.18550	3.82582	-0.34692
H	3.35411	3.24804	-1.93874
H	-5.92074	1.07828	-2.46738
H	-3.17950	-0.47723	0.46668
H	-7.73414	1.02964	-0.77135
H	-3.72192	-2.18662	1.78529
H	-4.48657	-2.37433	3.37316
H	-2.23259	-1.80800	3.78545
H	-3.22019	-0.39235	4.21591
H	-1.41094	0.96641	3.98667
H	-0.80921	1.31082	2.35400
H	-0.02111	-1.25033	3.90951
H	1.52154	0.82129	2.25985
H	2.27550	-1.83288	3.65833
H	3.18896	-0.33207	3.92050
H	4.27298	-2.87561	2.49572
H	5.02960	-1.39227	3.12553
H	4.89367	-2.16359	0.16494
H	6.28448	-2.35421	1.23402
H	-7.29095	0.14830	1.50627
H	6.30865	2.03754	0.95311

4·Cl, Conf1, 9:1 CH_3CN:H_2O

C	-0.40234	-0.55329	-4.16670
N	-1.34348	0.22628	-3.37690
N	0.94493	-0.01246	-4.02639
C	-2.04343	-0.24520	-2.34663
N	-2.79821	0.74298	-1.87364
C	-2.57363	1.88291	-2.63016
C	-1.66318	1.55666	-3.57648
C	1.63793	0.05855	-2.89013
N	2.83114	0.57906	-3.16564
C	2.90314	0.84740	-4.52271
C	1.71635	0.48014	-5.06100
C	3.86811	0.83371	-2.20202
C	4.00223	-0.04576	-1.13367
C	4.98198	0.21742	-0.17724
C	5.82076	1.32690	-0.33057
C	5.66542	2.17675	-1.41357
C	4.67477	1.94923	-2.36613
O	5.22482	-0.55132	0.91038
C	-3.69283	0.64484	-0.75384
C	-4.90136	1.33255	-0.79710
C	-3.31504	-0.11894	0.33631
C	-4.18084	-0.20794	1.42943
C	-5.39404	0.48230	1.42085
C	-5.73843	1.24402	0.30671
O	-3.75135	-0.98250	2.45008
C	-4.40697	-0.86442	3.71336
C	-3.57432	-1.61404	4.72845
O	-2.27451	-1.05835	4.82304
C	-1.27602	-1.78428	4.10751
C	-0.15705	-0.85073	3.76873
C	0.28062	-0.66225	2.52690
C	1.37308	0.29388	2.14807
O	2.38827	-0.32224	1.36746
C	3.21118	-1.19912	2.11161
C	4.36722	-1.64397	1.24778
H	-0.67097	-0.49589	-5.21832
H	-0.43010	-1.58182	-3.81445
H	-2.01154	-1.25763	-1.97336
H	-3.07024	2.81388	-2.41359
H	-1.20548	2.13921	-4.35967

H	1.28321	-0.23452	-1.91327
H	3.79014	1.25510	-4.97703
H	1.35253	0.50623	-6.07487
H	3.34535	-0.89925	-1.05290
H	6.31376	3.03884	-1.51421
H	4.52677	2.62969	-3.19515
H	-5.18098	1.90902	-1.67000
H	-2.35876	-0.62720	0.37488
H	-6.68528	1.77037	0.29903
H	-5.41446	-1.29022	3.66471
H	-4.47231	0.19296	3.98861
H	-3.52452	-2.67810	4.47433
H	-4.05997	-1.52009	5.70317
H	-1.69341	-2.20725	3.19028
H	-0.91468	-2.60752	4.73848
H	0.29781	-0.30862	4.59666
H	-0.17804	-1.21056	1.70421
H	1.80940	0.75314	3.04370
H	0.96517	1.08818	1.51703
H	2.65605	-2.08834	2.43688
H	3.59369	-0.68527	3.00335
H	4.02760	-2.16822	0.35244
H	4.99018	-2.32930	1.82321
H	-6.07045	0.42776	2.26364
H	6.58515	1.50613	0.41612

4·Cl, Conf2, 9:1 CH_3CN:H_2O

C	-0.74596	-0.82827	-4.23366
N	-1.64494	-0.05060	-3.39501
N	0.61308	-0.30414	-4.14173
C	-2.41437	-0.56314	-2.43561
N	-3.15596	0.41868	-1.93046
C	-2.84780	1.59884	-2.58908
C	-1.90331	1.30335	-3.51218
C	1.29917	-0.10522	-3.01720
N	2.51253	0.33300	-3.34660
C	2.60496	0.41097	-4.72610
C	1.41014	0.01444	-5.22384
C	3.53866	0.70439	-2.41198
C	3.62776	0.01618	-1.21439
C	4.57980	0.41838	-0.27548
C	5.45716	1.46342	-0.56980
C	5.35014	2.12110	-1.79198
C	4.38467	1.76374	-2.72414
O	4.58704	-0.27402	0.88431
C	-4.17326	0.25459	-0.92692
C	-5.36612	0.94071	-1.08504
C	-3.92582	-0.60506	0.13987
C	-4.94882	-0.81420	1.06584
C	-6.15970	-0.12305	0.93252
C	-6.35673	0.74898	-0.12415
O	-4.88223	-1.65808	2.11992
C	-3.74754	-2.50005	2.33114
C	-2.82245	-1.90857	3.36510
O	-2.29003	-0.69361	2.87419
C	-1.56471	0.03772	3.85615
C	-0.17334	-0.49202	4.04858
C	0.90807	0.28137	4.03651
C	2.30046	-0.21714	4.25823
O	3.09752	0.24328	3.17937
C	4.43375	-0.20857	3.24401
C	5.15954	0.33851	2.04272
H	-1.05575	-0.75217	-5.27304
H	-0.77400	-1.86231	-3.89756
H	-2.44758	-1.60114	-2.14134
H	-3.32021	2.53175	-2.33096
H	-1.38495	1.92229	-4.22646
H	0.92590	-0.24783	-2.01490
H	3.50814	0.72651	-5.22040
H	1.05467	-0.08333	-6.23628
H	2.97386	-0.81611	-0.98290
H	6.02695	2.93700	-2.01525
H	4.28316	2.30419	-3.65659
H	-5.52653	1.58811	-1.93777
H	-2.95394	-1.06603	0.24777
H	-7.30052	1.27249	-0.21789
H	-3.23068	-2.70856	1.39344
H	-4.14500	-3.44046	2.71588
H	-2.03153	-2.63785	3.58121
H	-3.38266	-1.72161	4.29028
H	-2.11915	0.01257	4.80366
H	-1.52573	1.07346	3.51322
H	-0.07055	-1.56196	4.22311
H	0.80870	1.35187	3.86082
H	2.31553	-1.31342	4.30643
H	2.70606	0.17217	5.20321
H	4.46769	-1.30578	3.24570
H	4.92484	0.15578	4.15567
H	6.22787	0.11207	2.09859
H	5.02017	1.42193	1.99768
H	-6.93437	-0.29115	1.67121
H	6.21804	1.76119	0.14004

4·Cl, Conf3, 9:1 CH_3CN:H_2O

C	-0.42714	-0.80747	-4.00818
N	-1.26275	0.04759	-3.18917
N	0.97565	-0.39839	-3.89661
C	-1.77421	-0.30097	-2.00806
N	-2.45096	0.73699	-1.52874
C	-2.36851	1.78614	-2.43120
C	-1.62265	1.35331	-3.47412
C	1.59367	-0.01221	-2.78252
N	2.87551	0.19926	-3.07312
C	3.08324	-0.06397	-4.41501
C	1.88806	-0.43830	-4.93206
C	3.86250	0.66181	-2.13671
C	3.80001	0.18073	-0.83319
C	4.72088	0.66463	0.09373
C	5.69313	1.58813	-0.30932
C	5.73350	2.03416	-1.62009
C	4.80849	1.58156	-2.55925
O	4.76757	0.29612	1.39437
C	-3.12716	0.75851	-0.26183
C	-3.07237	1.91114	0.51180
C	-3.77803	-0.39024	0.16126
C	-4.38228	-0.39275	1.41567
C	-4.35449	0.75424	2.21000
C	-3.70368	1.89450	1.75073
O	-5.05784	-1.51916	1.78146
C	-4.74481	-2.08689	3.05987
C	-3.56828	-3.03867	2.93244
O	-2.42151	-2.41832	2.38283
C	-1.73714	-1.56486	3.29152
C	-0.58846	-0.93244	2.57074
C	-0.41924	0.38468	2.49803
C	0.71941	1.08745	1.81373
O	1.77730	0.24347	1.40564
C	2.62216	-0.17041	2.46717
C	3.90981	-0.72662	1.90891
H	-0.71644	-0.70995	-5.05180
H	-0.54144	-1.83367	-3.66649
H	-1.64135	-1.25673	-1.52390
H	-2.86359	2.72584	-2.25292
H	-1.32327	1.83668	-4.38956
H	1.13863	0.13356	-1.81446
H	4.05536	0.02966	-4.86880
H	1.60186	-0.73341	-5.92798
H	3.03830	-0.53281	-0.55429
H	6.48694	2.75358	-1.91725
H	4.81353	1.94846	-3.57819
H	-2.54044	2.78832	0.16419
H	-3.82119	-1.27883	-0.45719
H	-3.68247	2.78273	2.37076
H	-5.62722	-2.64480	3.37517
H	-4.55936	-1.29970	3.79301
H	-3.83283	-3.84679	2.24773
H	-3.34724	-3.47091	3.91775
H	-1.38037	-2.16494	4.14055
H	-2.40320	-0.78615	3.68058
H	0.13093	-1.60773	2.11181
H	-1.15215	1.04507	2.95986
H	1.10438	1.87956	2.46972
H	0.34560	1.57798	0.90832
H	2.14375	-0.94865	3.07241
H	2.84898	0.68228	3.11921
H	3.72596	-1.49732	1.15662
H	4.47170	-1.17807	2.72726
H	-4.85020	0.76144	3.17339
H	6.40766	1.94251	0.42408

4·Cl, Conf4, 9:1 CH_3CN:H_2O

C	-0.42993	-0.89875	-3.58976
N	-1.61936	-0.17665	-3.15487
N	0.76420	-0.09149	-3.38470
C	-2.40395	-0.54467	-2.14440
N	-3.39821	0.33498	-2.04931
C	-3.24108	1.29729	-3.03454
C	-2.12783	0.97224	-3.73175
C	1.48980	-0.04819	-2.26575
N	2.48323	0.81520	-2.45463
C	2.38884	1.34471	-3.73132
C	1.31010	0.77427	-4.31507
C	3.51217	1.14624	-1.50560
C	4.11654	0.11687	-0.79375
C	5.13314	0.44625	0.10367
C	5.51882	1.78226	0.25631
C	4.89305	2.78212	-0.47108
C	3.87062	2.47798	-1.36581
O	5.85302	-0.45163	0.81830
C	-4.46549	0.27890	-1.08836
C	-5.72595	0.72030	-1.45969
C	-4.18356	-0.21186	0.18199
C	-5.22220	-0.27864	1.10916
C	-6.49843	0.17875	0.76616
C	-6.73918	0.67608	-0.50454
O	-5.07126	-0.73898	2.37397
C	-4.02480	-1.66610	2.68406
C	-2.85931	-1.01109	3.38200
O	-2.14519	-0.20284	2.46526
C	-1.07137	0.51824	3.05965
C	0.12861	-0.34594	3.31585
C	1.34801	-0.05821	2.86959
C	2.56175	-0.86356	3.20510
O	3.30301	-1.09665	2.01738
C	4.48898	-1.82349	2.26893
C	5.37093	-1.77771	1.04604
H	-0.51153	-1.11564	-4.65169
H	-0.35070	-1.81553	-3.01031
H	-2.26471	-1.41878	-1.52702
H	-3.92248	2.12475	-3.13784
H	-1.64601	1.45167	-4.56834

H	1.30095	-0.61094	-1.36414
H	3.11001	2.05291	-4.10331
H	0.88815	0.88457	-5.30061
H	3.80345	-0.90381	-0.96256
H	5.19743	3.81304	-0.33644
H	3.36195	3.25050	-1.92871
H	-5.92060	1.07650	-2.46327
H	-3.17532	-0.48642	0.46264
H	-7.73323	1.01760	-0.76681
H	-3.70273	-2.19281	1.78209
H	-4.47090	-2.39084	3.36716
H	-2.22294	-1.80666	3.78765
H	-3.22316	-0.39962	4.21761
H	-1.42010	0.97242	3.99680
H	-0.81405	1.32129	2.36634
H	-0.01869	-1.23418	3.92812
H	1.51468	0.82984	2.26037
H	2.27698	-1.81450	3.67349
H	3.19324	-0.31175	3.91625
H	4.25959	-2.87000	2.51023
H	5.02645	-1.38273	3.11851
H	4.86596	-2.17889	0.16640
H	6.26124	-2.38009	1.22811
H	-7.28718	0.12807	1.50722
H	6.31621	2.01373	0.95252

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