Supporting Information for:

Exploring Anion-Induced Conformational Flexibility and Molecular Switching in a Series of Heteroaryl-Urea Receptors

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Experimental Procedures

General. Tetrabutylammonium salts were dried at 50 °C under vacuum and stored in a dessicator over $CaCO_3$. All other materials were obtained from TCI-America, Sigma-Aldrich, or Acros and used as received. Reactions were performed under an inert N_2 atmosphere in dried glassware. ^1H and ^{13}C NMR spectra were recorded using a Bruker Avance III HD 600 (^1H: 600.0 MHz; ^{13}C: 150.9 MHz), Agilent VNMRS 600 (^1H: 600.0 MHz; ^{13}C: 150.9 MHz), Varian Inova 500 (^1H: 500.1 MHz; ^{13}C: 121.4 MHz) or Varian Inova 300 (^1H: 299.9 MHz) spectrometer. Chemical shifts (δ) are reported in ppm downfield shift of tetramethylsilane (δ_H 0.00) and referenced to residual non-deuterated solvent DMSO (DMSO-d_6: δ_H 2.50 ppm, δ_C 39.52 ppm) or $CHCl_3$ ($CDCl_3$: δ_H 7.26 ppm). Mixed solvent systems were referenced to the most abundant solvent. $CDCl_3$ was passed through a column of activated basic alumina prior to use. All NMR spectra were processed using MestReNova NMR processing software. Solutions for UV-Vis spectroscopy were prepared using spectroscopy grade solvents. All UV/Vis spectra were obtained via an HP 8453 spectrometer using an optical filter < 265 nm. Spectra of pure solvent matrix served as blank spectra.

NMR Titrations. Solutions of **2** and **3** were prepared using 10% DMSO-d_6/$CDCl_3$ in a volumetric flask to a final concentration of ranging from 0.0003-0.001 M and 0.0010-0.0018 M, respectively. In each case, 500 μL of this solution was transferred to an NMR tube, and the remainder of the receptor solution was used to generate the guest tetrabutylammonium salt stock solutions to maintain a constant host concentration throughout the titrations. Aliquots of the guest solutions were added via Hamilton gas tight syringes to the host solution in the NMR tube, and a spectrum was obtain via a Varian Inova 500, an Agilent VNMRS 600, or Bruker Avance III 600 spectrometer at 298 K after thorough mixing. Association constants (K_a) were calculated by non-linear curve fitting of the obtained titration isotherms using HypNMR 2006.[1] The reported association constants were calculated from the downfield shifting of the urea proton resonances in all cases. All titrations were performed in triplicate.

UV/Vis Titrations. Stock solutions of **2** and **3** were prepared in 10% DMSO/$CHCl_3$. An aliquot of the stock receptor solution was diluted with the same solvent matrix to final concentrations of approximately 11-14 μM and 25-28 μM, respectively. Quartz cuvettes were

charged with 2 mL of receptor solution. To maintain a constant receptor concentration throughout titrations the receptor solution was used to prepare stock and final guest tetrabutylammonium salt solutions. Guest solutions were added repeatedly in microliter aliquots via Hamilton gas tight syringes, and spectra were obtained upon solution equilibrium. Association constants (K_a) were calculated by non-linear curve fitting of the obtained titration isotherms using HyperQuad 2006.[2] In all cases wavelength ranges from 355-410 nm for **2** and 360-410 nm for **3** were used in the determination of association constants.

X-Ray Crystallography. Diffraction intensities for **2** and **3** were collected at –193(2) and 100(2) K on a Bruker Apex2 CCD diffractometer using CuKα radiation λ= 1.54178 Å and MoKα radiation λ= 0.71073 Å, respectively. Space groups were determined based on systematic absences (**3**) and intensity statistics (**2**). Absorption corrections were applied by SADABS.[3] Structures were solved by direct methods and Fourier techniques and refined on F^2 using full matrix least-squares procedures. All non-H atoms in both structures were found from the residual density maps and refined with isotropic thermal parameters. Besides the main molecules the crystal structure of **3** has solvent water molecule and the structure of **2** has two methanol and one CH_2Cl_2 molecules. The last one is disordered over two positions and the refinement shown that the position of this solvent molecule is not fully occupied. Checking different values of occupation factor for this molecule showed that the total occupation factor of the disordered CH_2Cl_2 molecule of 0.69 provides the best results. Thus the total occupation of the disordered CH_2Cl_2 molecule was fixed at this value in the final refinement of **2**. All calculations were performed by the Bruker SHELXTL (v. 6.10) package.[4]

Calculated Structures. Receptor:anion complexes were started in the proposed conformations and allowed to find a local minima. All structures were optimized with Gaussian 09[6] using ωB97X-D/6-31G(d,p)[5,6] with a DMSO solvent field applied. Upon successful convergence, the energy of each structure was calculated at the same level of theory. Relative energies were calculated including the zero-point energies of the optimized structures

Aniline 4. A solution of 2-bromopyridine (0.205 g, 1.3 mmol) in *i*Pr_2NH (30 mL) and THF (20 mL) was purged with N_2 for 30 min. CuI (0.017 g, 0.089 mmol, 7 mol%) and $Pd(PPh_3)_4$ (0.06 g, 0.052 mmol, 4 mol%) were added to the solution, and the mixture was purged with N_2

for an additional 20 min. A degassed solution of 4-*t*-butyl-2-ethynylaniline (0.227 g, 1.31 mmol) in THF (10 mL) was transferred via cannula to the bromopyridine solution, and the reaction was stirred at 25 °C for 4 h. Upon completion, the reaction mixture was concentrated in vacuo, and the resulting dark brown residue was purified via flash column chromatography (4:1 CH_2Cl_2/hexanes) to afforded dianiline **4** (0.228 g, 89 %) as a light brown powder. ^{1}H NMR (600 MHz, CD_2Cl_2, 25 °C, TMS) δ 8.60 (d, *J* = 4.3 Hz, 1H), 7.68 (td, *J* = 7.7, 1.8 Hz, 1H), 7.53 (d, *J* = 7.8 Hz, 1H), 7.44 (d, *J* = 2.3 Hz, 1H), 7.26–7.20 (m, 2H), 6.71 (d, *J* = 8.5 Hz, 1H), 4.44 (s, 2H), 1.29 (s, 9H); ^{13}C NMR (151 MHz, CD_2Cl_2, 25 °C, TMS) δ 150.56, 147.06, 144.11, 141.08, 136.65, 129.52, 128.53, 127.40, 123.12, 114.80, 106.37, 94.24, 87.03, 34.32, 31.67; HRMS (ESI) for $C_{17}H_{19}N_2^+$: calcd 251.1548, found 251.1538.

Dianiline 5. A solution of 2,9-diiodophenanthroline[7] (0.085g, 0.46 mmol) in *i*Pr_2NH (70 mL) and THF (50 mL) and purged with N_2 for 30 min. CuI (0.096 g, 0.51 mmol, 110 mol%) and $Pd(PPh_3)_4$ (0.053 g, 0.046 mmol, 10 mol%) were added to the solution, and the mixture was purged with N_2 for an additional 20 min. A degassed solution of 4-*t*-butyl-2-ethynylaniline (0.161 g, 0.93 mmol) in THF (20 mL) was then transferred via cannula to the iodophenanthroline solution. After stirring overnight at 25 °C, the reaction mixture was concentrated in vacuo to yield a dark red residue. A small portion of THF was added to the residue and the solution was washed with a basic solution of EDTA until the aqueous layer no longer generated a blue hue. The resulting organic layer was diluted with Et_2O, washed with brine, dried ($MgSO_4$) and concentrated under reduced pressure. The resulting brown solid was sonicated in a small amount of hexanes:ethyl acetate (5:1) and filtered to afford the phenanthroline bis-aniline **5** (0.178 g, 0.34 mmol, 74%) as a dark yellow solid. ^{1}H NMR (500 MHz, CD_2Cl_2, 25 °C, TMS) δ 8.27 (d, *J* = 8.3 Hz, 2H), 7.86 (d, *J* = 8.2 Hz, 2H), 7.83 (s, 2H), 7.58 (d, *J* = 1.8 Hz, 2H), 7.24 (dd, *J* = 8.5, 2.0 Hz, 2H), 6.69 (d, *J* = 8.5 Hz, 2H), 4.57 (s, 4H), 1.31 (s, 18H); ^{13}C NMR (126 MHz, CD_2Cl_2, 25°C, TMS) δ 147.40, 146.33, 144.12, 141.20, 136.72, 130.14, 128.86, 128.44, 127.17, 126.80, 114.84, 106.32, 95.05, 88.59, 34.42, 31.71; HRMS (ESI) for $C_{36}H_{35}N_4^+$: calcd 523.2862, found 523.2843.

Receptor 3. A solution of aniline **4** (0.250 g, 1.0 mmol) in toluene (40 mL) was purged with N_2 for 30 min. 4-Nitrophenylisocyanate (0.180 g, 1.1 mmol) was added to the solution, and the mixture was stirred overnight at 25 °C under an inert atmosphere. The solvent was

evaporated to yield a dark yellow solid that was then suspended in a small amount of EtOH and sonicated in a heated water bath for 1 h. The resulting light brown solid was filtered yielding **3** (0.311 g, 0.75 mmol, 75%). ^{1}H NMR (600 MHz, 10% DMSO-d_6/$CDCl_3$, 25 °C, TMS) δ 9.56 (s, 1H), 8.56 (d, J = 4.3 Hz, 1H), 8.37 (s, 1H), 8.26 (d, J = 8.8 Hz, 1H), 8.17 (d, J = 9.2 Hz, 2H), 7.80 (td, J = 7.7, 1.6 Hz, 1H), 7.71 (d, J = 9.2 Hz, 2H), 7.61 (d, J = 7.8 Hz, 1H), 7.52 (d, J = 2.3 Hz, 1H), 7.45 (dd, J = 8.8, 2.3 Hz, 1H), 7.35 (dd, J = 7.0, 5.5 Hz, 1H), 1.33 (s, 9H); ^{13}C NMR (126 MHz, DMSO-d_6, 25 °C, TMS) δ 151.80, 150.08, 146.14, 145.51, 142.30, 141.16, 137.36, 136.74, 129.11, 127.78, 127.41, 125.19, 123.67, 120.42, 117.57, 111.24, 94.26, 84.82, 34.04, 30.95; HRMS (ESI) for $C_{24}H_{23}N_4O_3^+$: calcd 415.1770, found 415.1778.

Receptor 2. A solution of dianiline **5** (0.042g, 0.08 mmol) in toluene (60 mL) was purged with N_2 for 30 min. 4-Nitrophenylisocyanate (0.033 g, 0.20 mmol) was added to the solution, and the mixture was stirred overnight at 25 °C under an inert atmosphere. The solvent was evaporated to yield a bright yellow solid that was then suspended in a small amount of EtOH and sonicated in a heated water bath for 1 h. The resulting pale yellow solid was filtered yielding **2** (0.056 g, 0.066 mmol, 82%). ^{1}H NMR (500 MHz, DMSO-d_6, 25 °C, TMS) δ 10.23 (s, 2H), 8.70 (s, 2H), 8.62 (d, J = 8.3 Hz, 2H), 8.17 (d, J = 8.3 Hz, 2H), 8.13 (d, J = 9.2 Hz, 4H), 8.09 (s, 2H), 8.00 (d, J = 8.8 Hz, 2H), 7.70 (dd, J = 5.8, 3.3 Hz, 6H), 7.51 (dd, J = 8.8, 2.2 Hz, 2H), 1.30 (s, 18H); ^{13}C NMR (126 MHz, DMSO-d_6, 25 °C, TMS) δ 151.83, 146.14, 145.63, 144.93, 142.39, 141.14, 137.69, 136.99, 129.45, 128.12, 127.78, 127.28, 127.19, 125.15, 120.48, 117.53, 111.09, 94.95, 86.50, 34.10, 30.96; HRMS (ESI) for $C_{50}H_{43}N_8O_6^+$: calcd 851.3306, found 851.3335.

1D NMR Spectroscopic Data

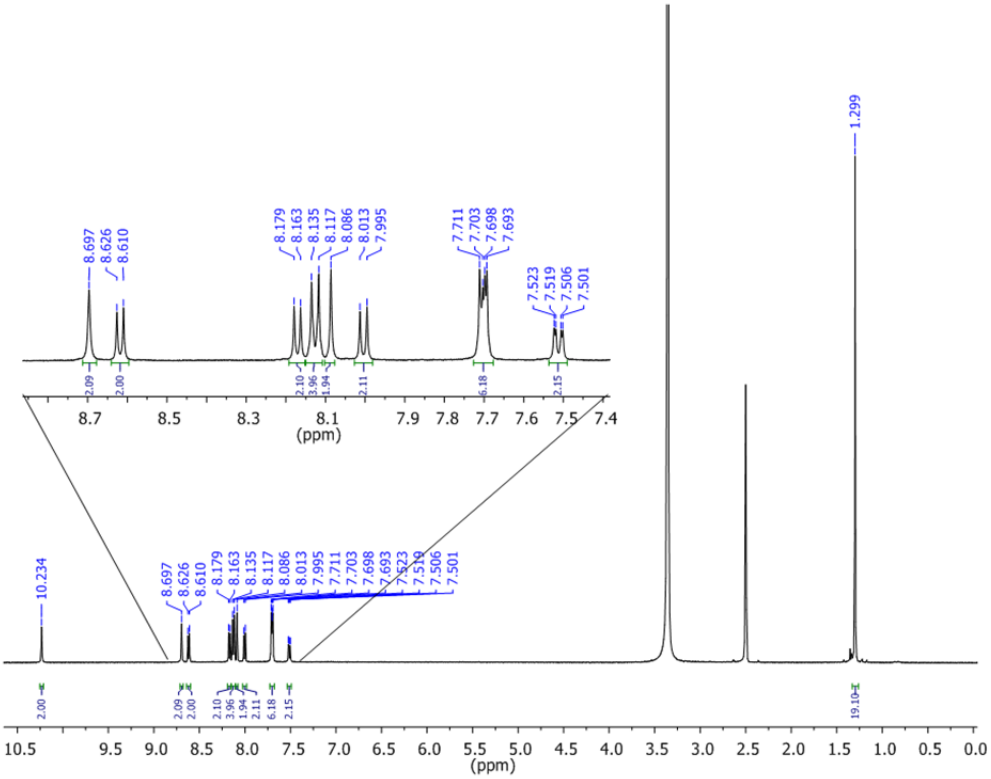

Fig. S1 ^{1}H NMR spectra of **2** in DMSO-d_6, 500 MHz.

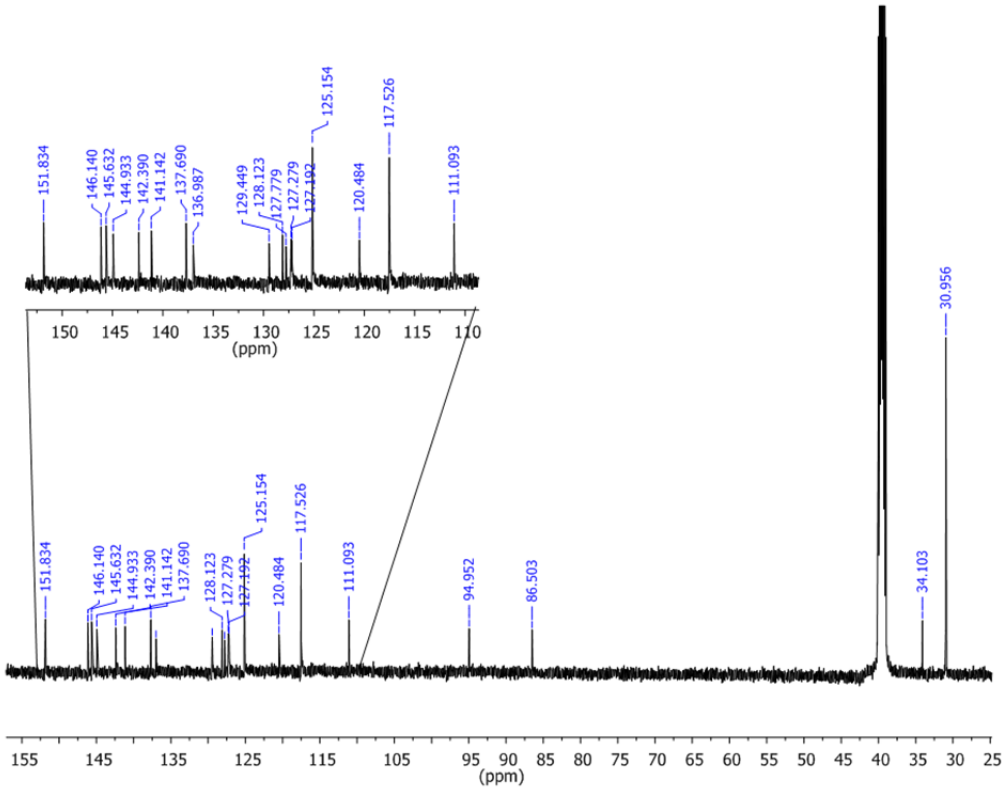

Fig. S2 ^{13}C NMR spectrum of **2** in DMSO-d_6, 121.4 MHz.

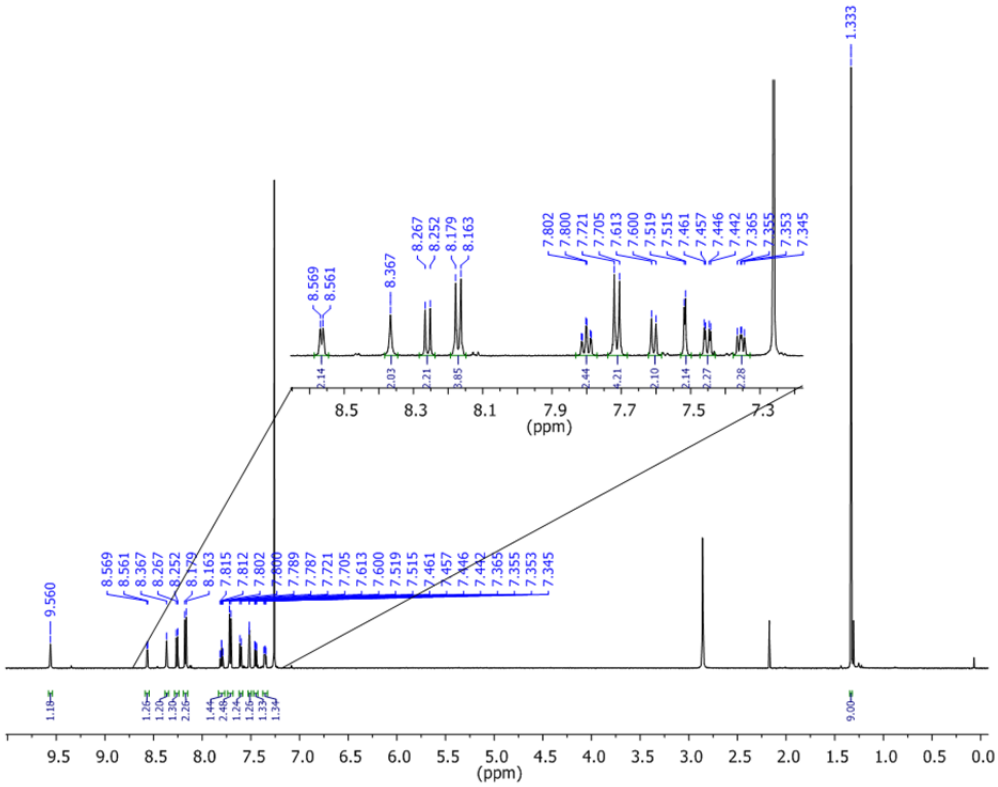

Fig. S3 ^{1}H NMR spectra of **3** in 10% DMSO-d_6/$CDCl_3$, 600 MHz.

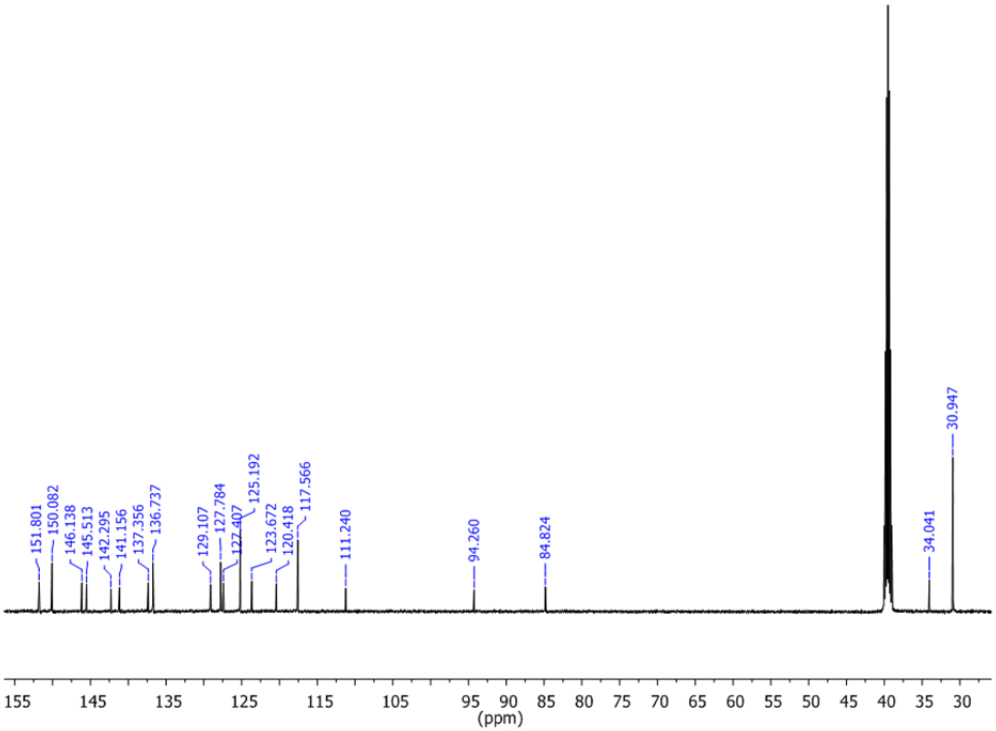

Fig. S4 ^{13}C NMR spectrum of **3** in DMSO-d_6, 121.4 MHz.

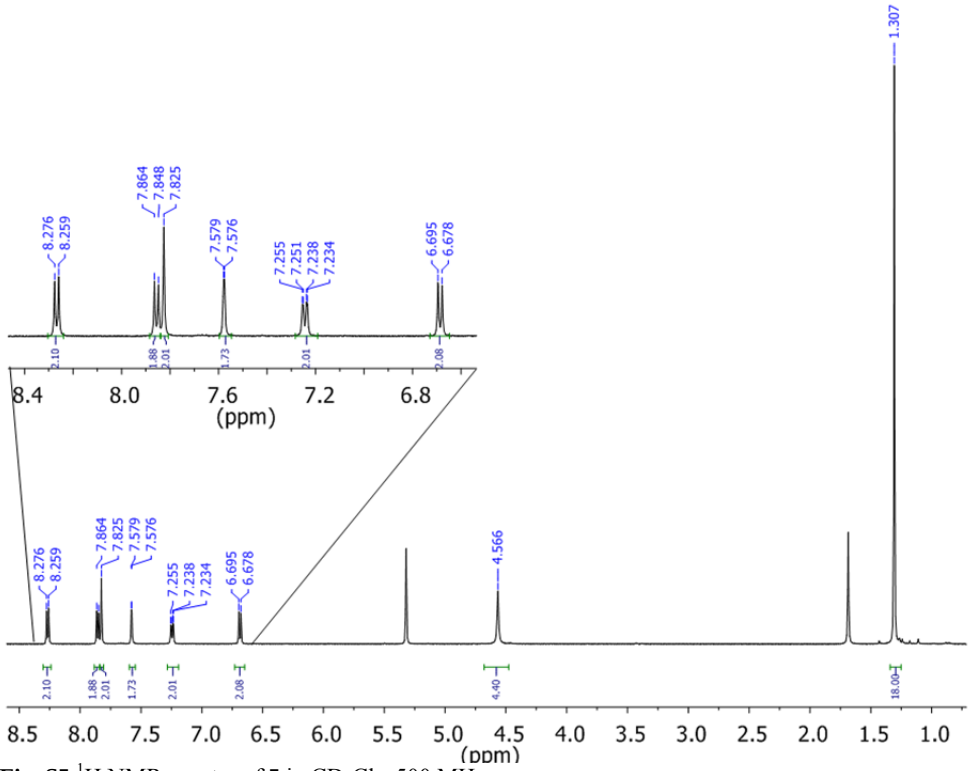

Fig. S5 ^{1}H NMR spectra of **5** in CD_2Cl_2, 500 MHz.

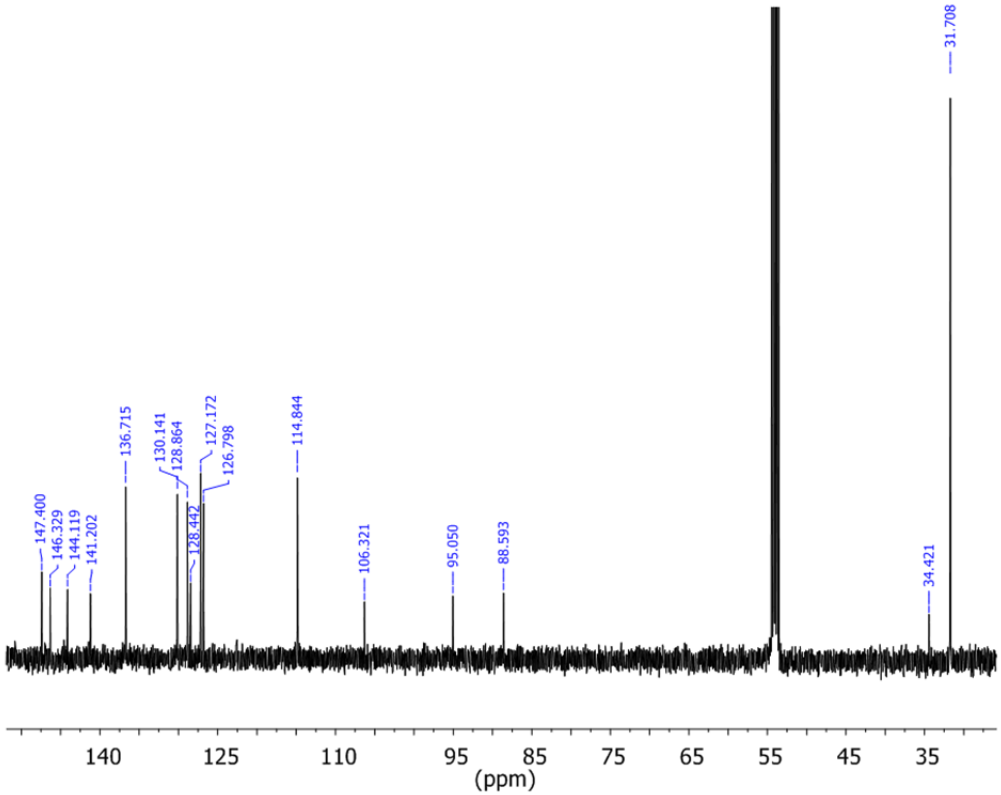

Fig. S6 ^{13}C NMR spectrum of **5** in CD_2Cl_2, 126 MHz

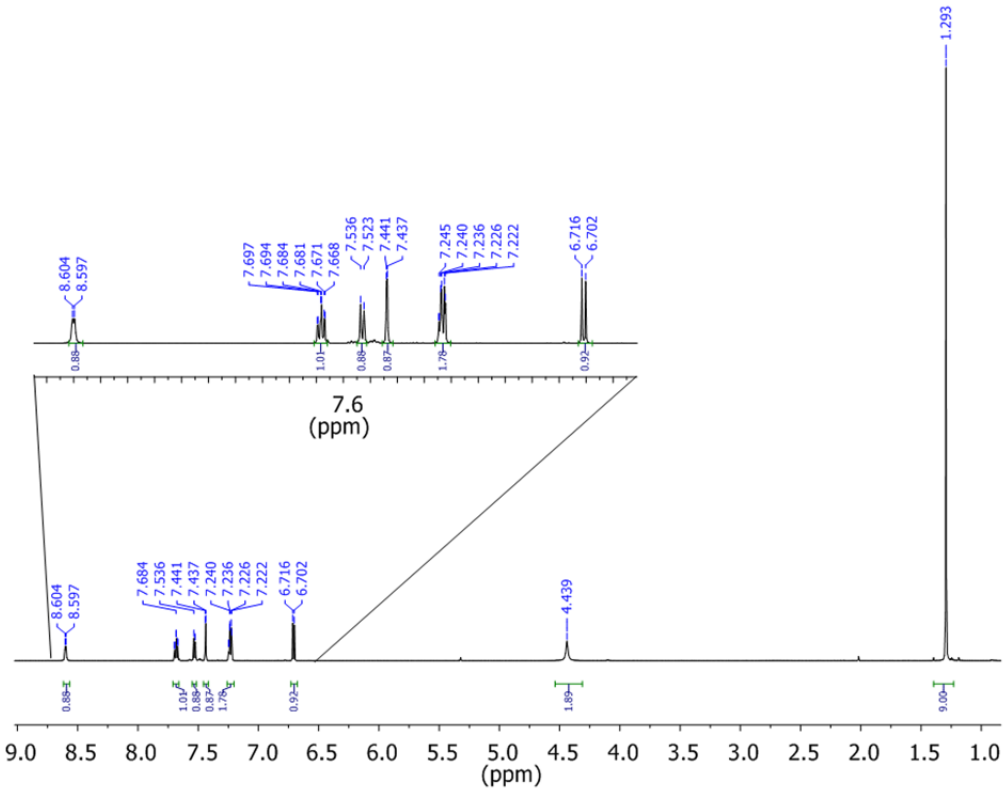

Fig. S7 ^{1}H NMR spectra of **4** in CD_2Cl_2, 600 MHz.

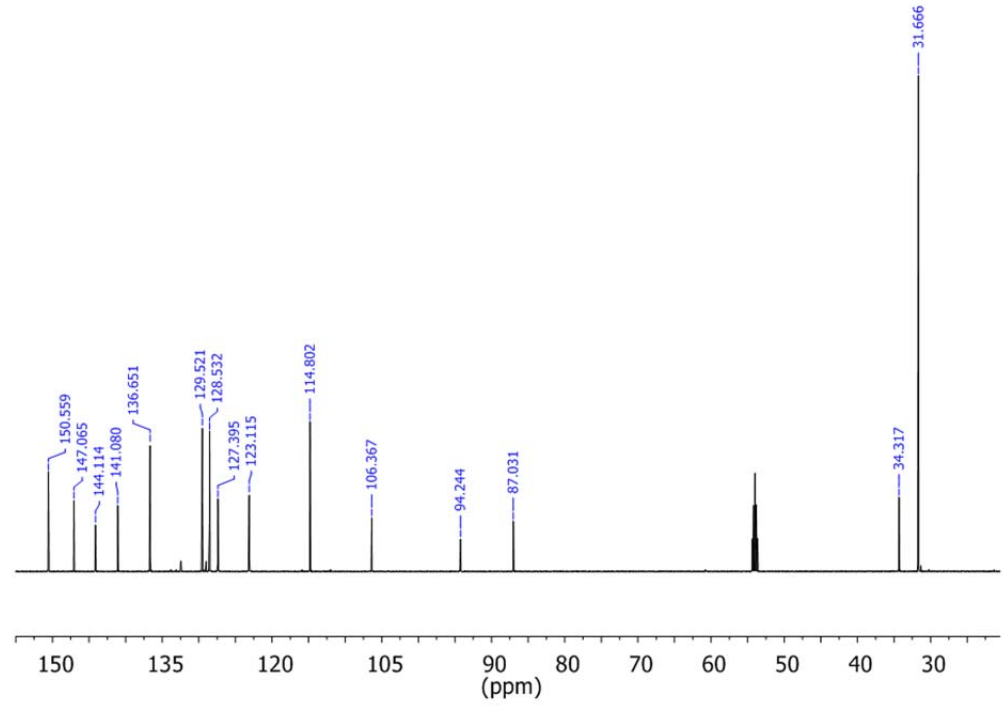

Fig. S8 ^{13}C NMR spectrum of **6** in CD_2Cl_2, 151 MHz.

2-D NMR spectroscopic data

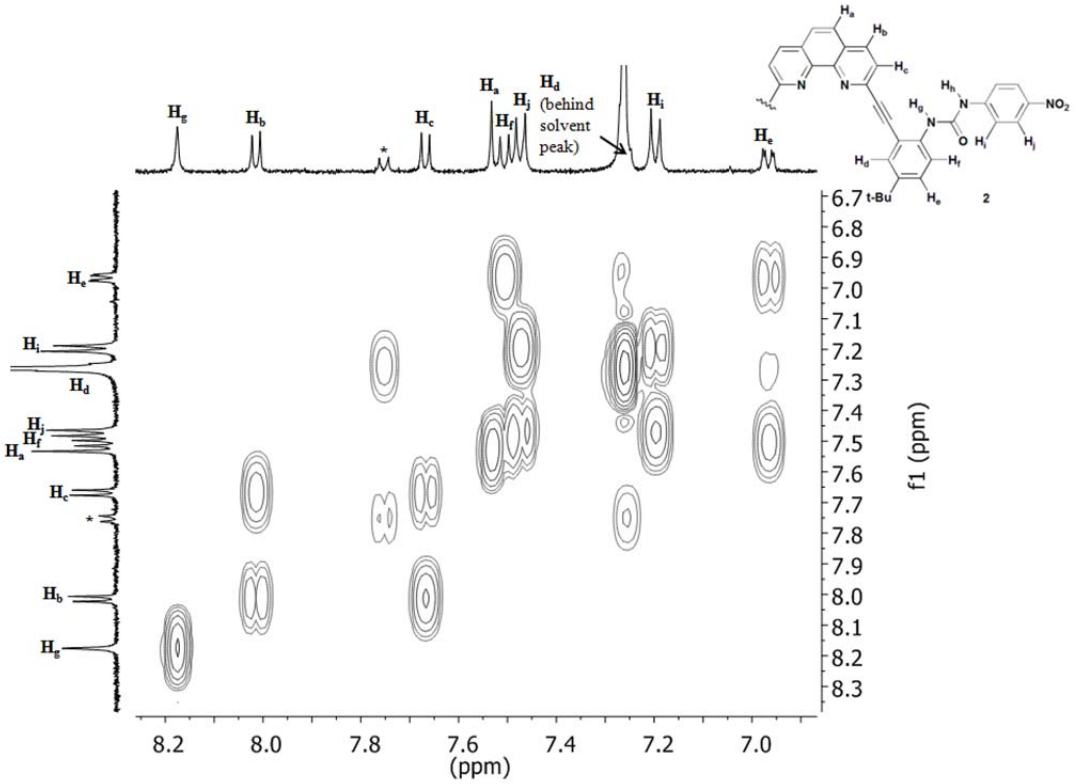

Fig. S9 ^{1}H-^{1}H gradient COSY NMR spectra of **2** in 10% DMSO-d_6/$CDCl_3$, 500 MHz. * = minor impurity.

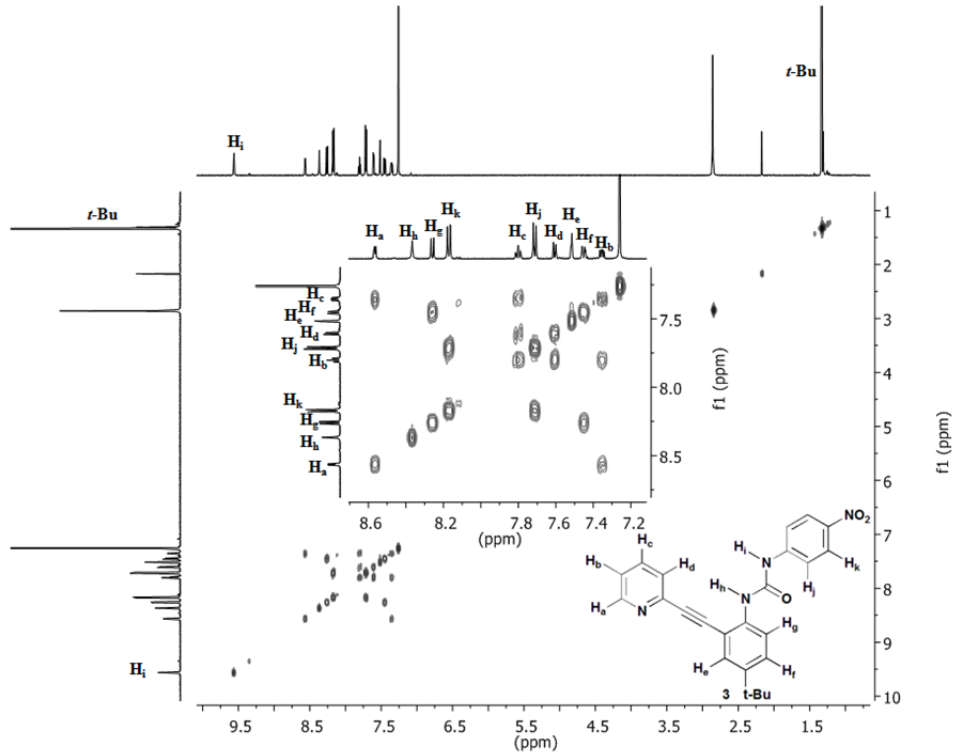

Fig. S10 ^{1}H-^{1}H gradient COSY NMR spectra of **3** in 10% DMSO-d_6/$CDCl_3$, 600 MHz.

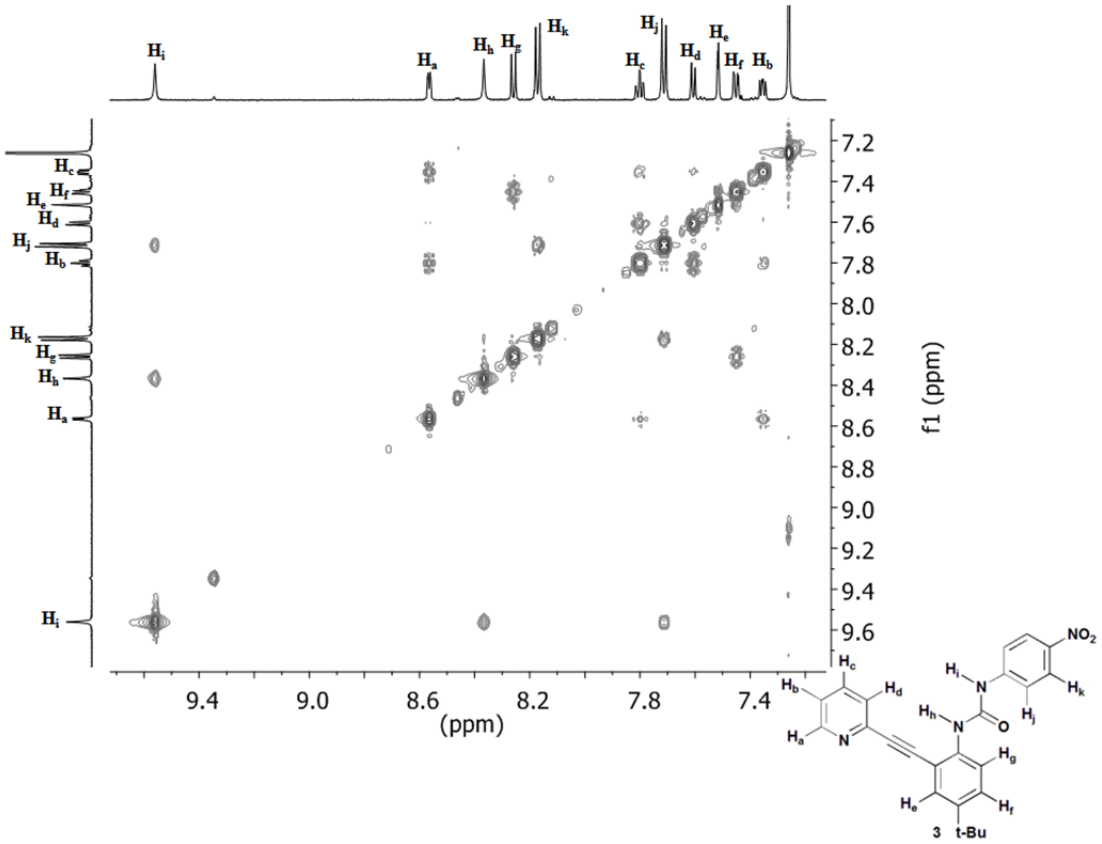

Fig. S11 NOESY NMR spectra of **3** in 10% DMSO-d_6/$CDCl_3$, 600 MHz.

Representative Titration Data

Fit Binding Curves

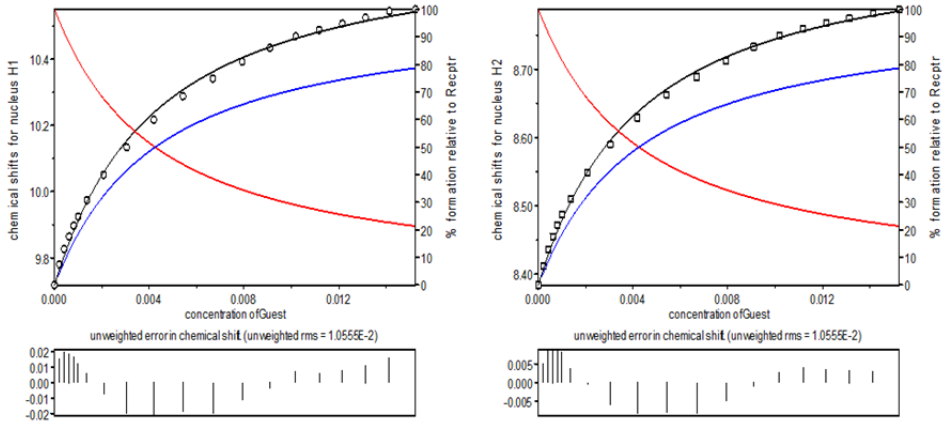

Fig. S12 Representative fit titration curves of **2**·Cl^-.

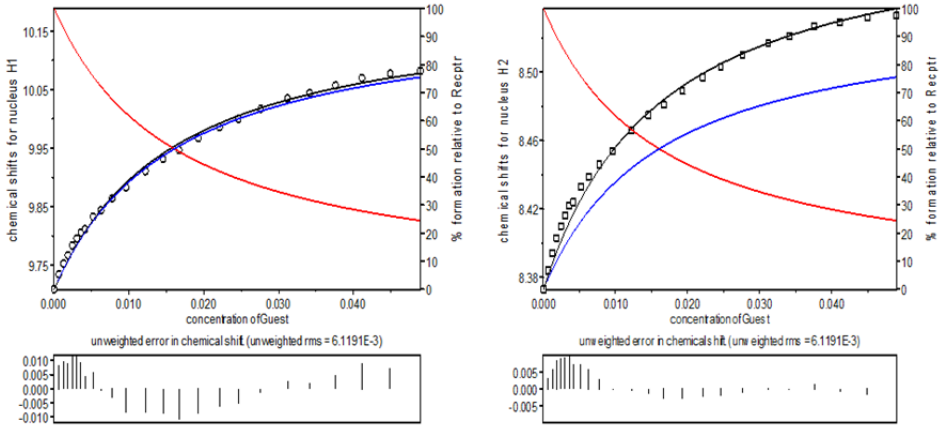

Fig. S13 Representative fit titration curves of **2**·Br^-.

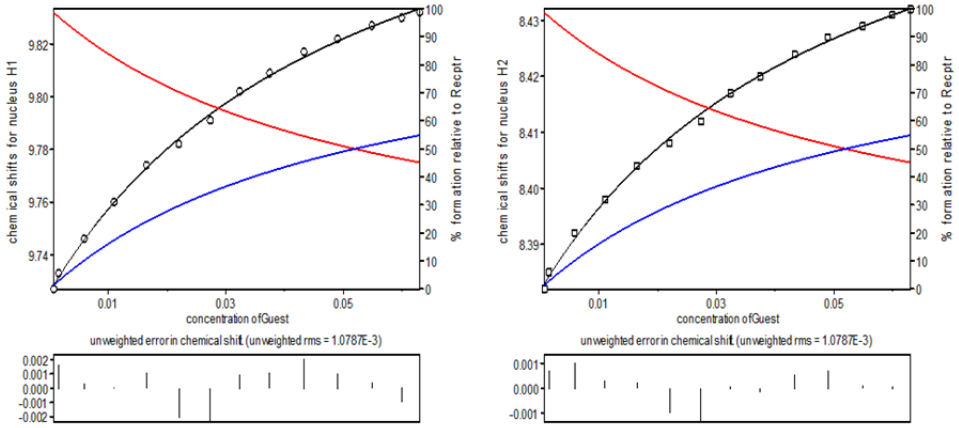

Fig. S14 Representative fit titration curves of **2**·I^-.

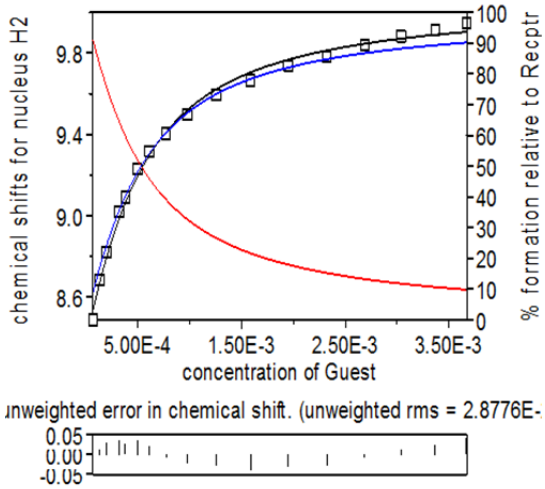

Fig. S15 Representative fit titration curve of **2**·OAc^-.

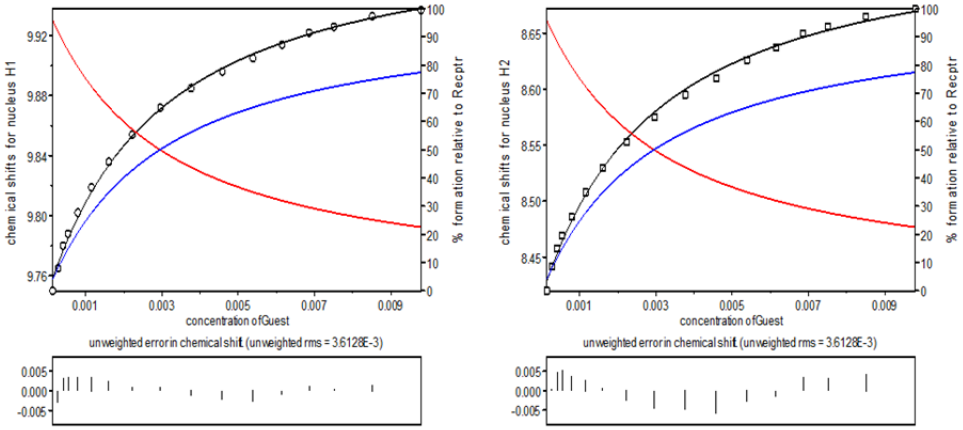

Fig. S16 Representative fit titration curves of **2**·HSO_4^-.

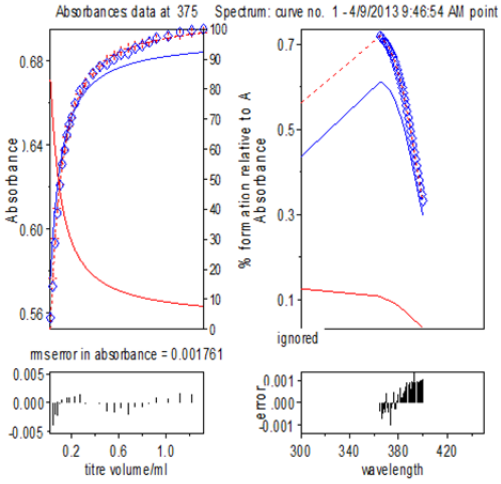

Fig. S17 Representative fit titration curve of **2**·$H_2PO_4^-$.

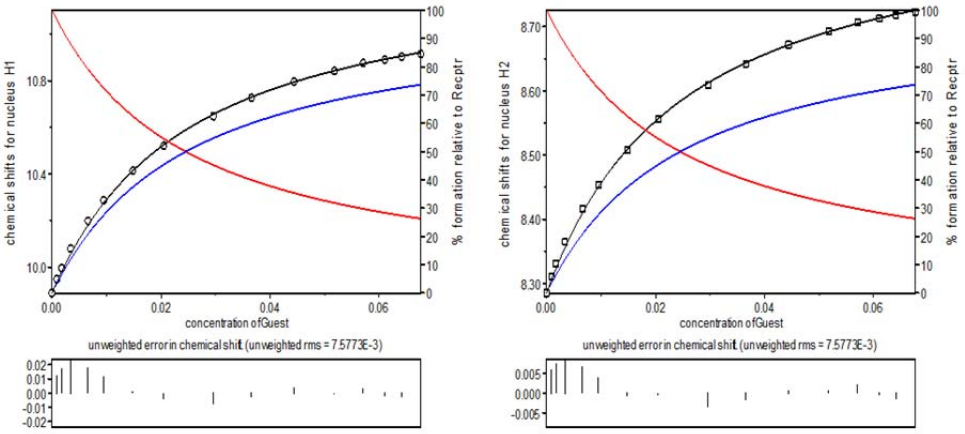

Fig. S18 Representative fit titration curves of **3**·Cl^-.

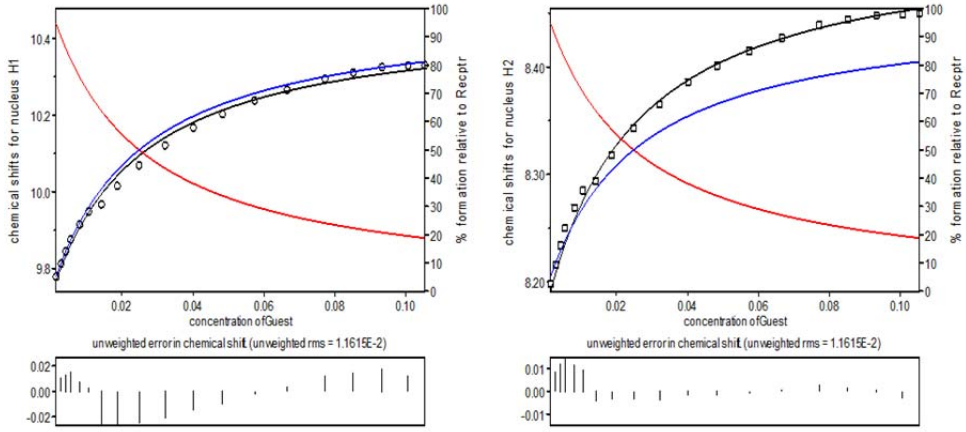

Fig. S19 Representative fit titration curves of **3**·Br^-.

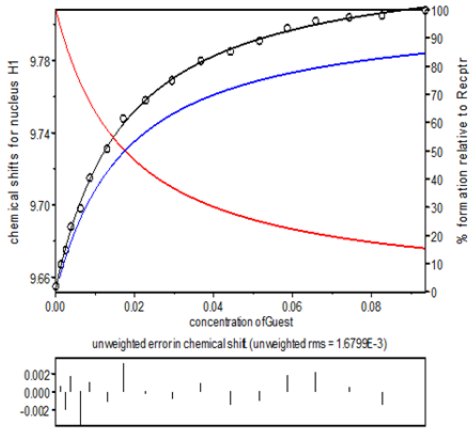

Fig. S20 Representative fit titration curve of **3**·I^-.

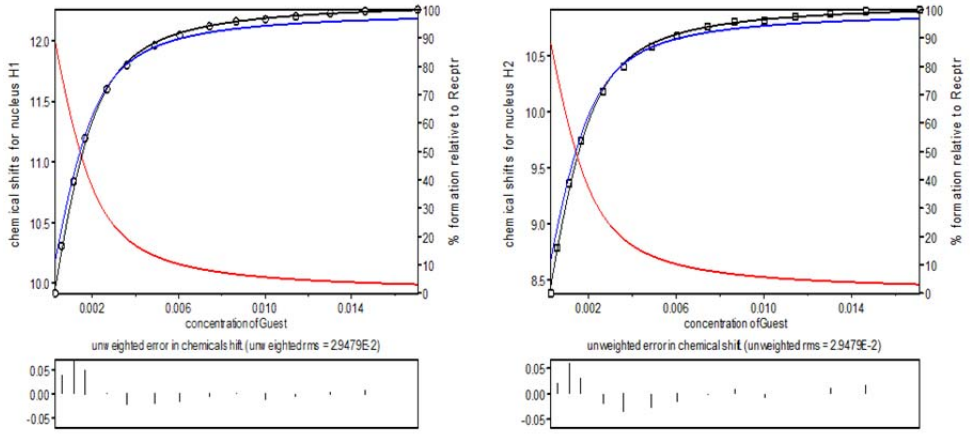

Fig. S21 Representative fit titration curves of **3**·OAc^-.

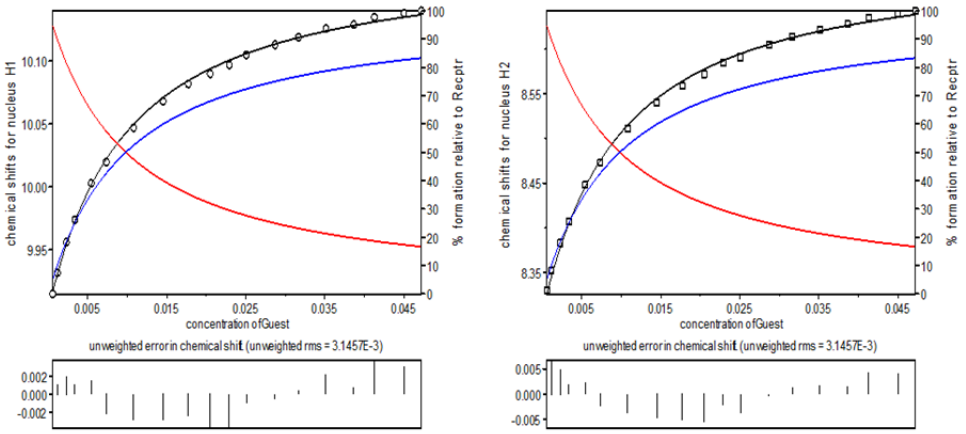

Fig. S22 Representative fit titration curves of **3**·HSO_4^-.

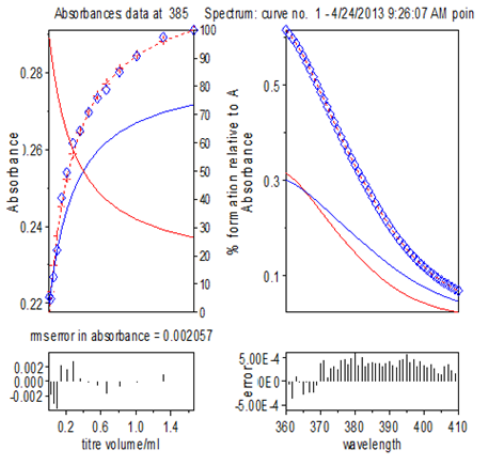

Fig. S23 Representative fit titration curve of **3**·$H_2PO_4^-$.

Stacked Spectra

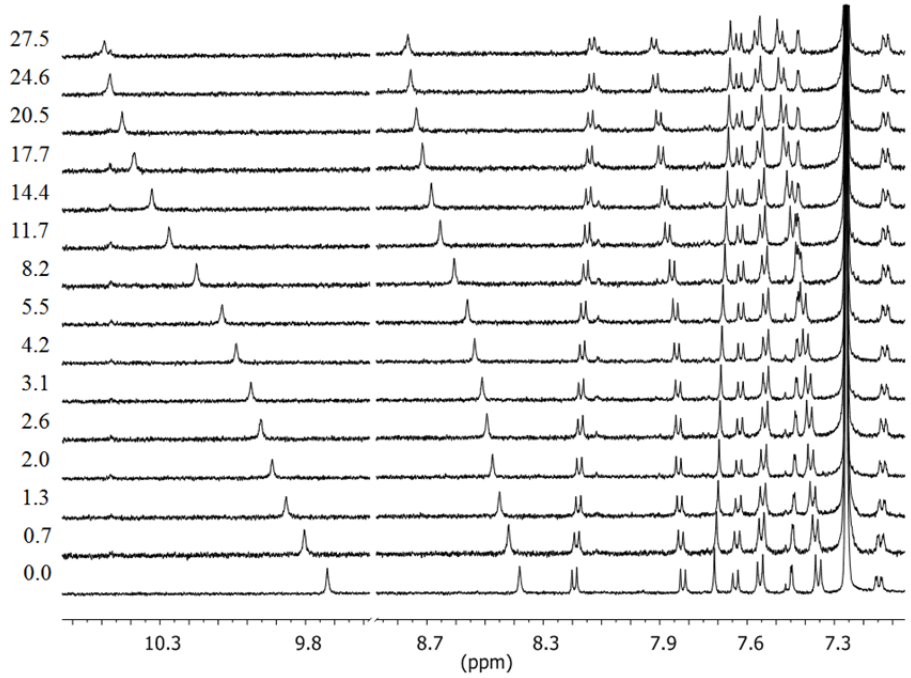

Fig. S24 Representative stacked ^{1}H NMR titration data for **2**·Cl^{-}. [Guest]/[Host] listed on left.

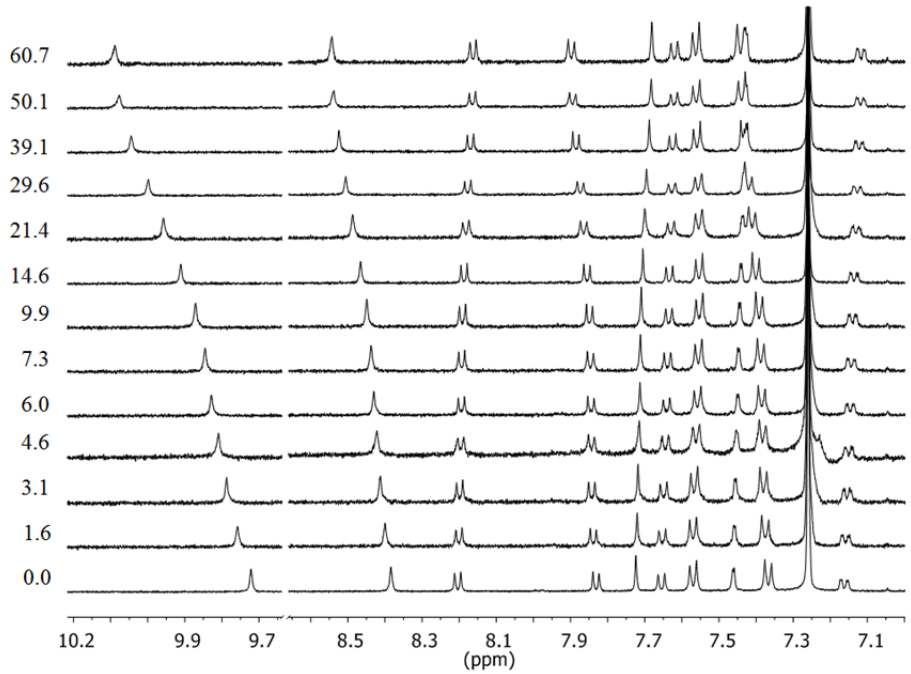

Fig. S25 Representative stacked ^{1}H NMR titration data for **2**·Br^{-}. [Guest]/[Host] listed on left.

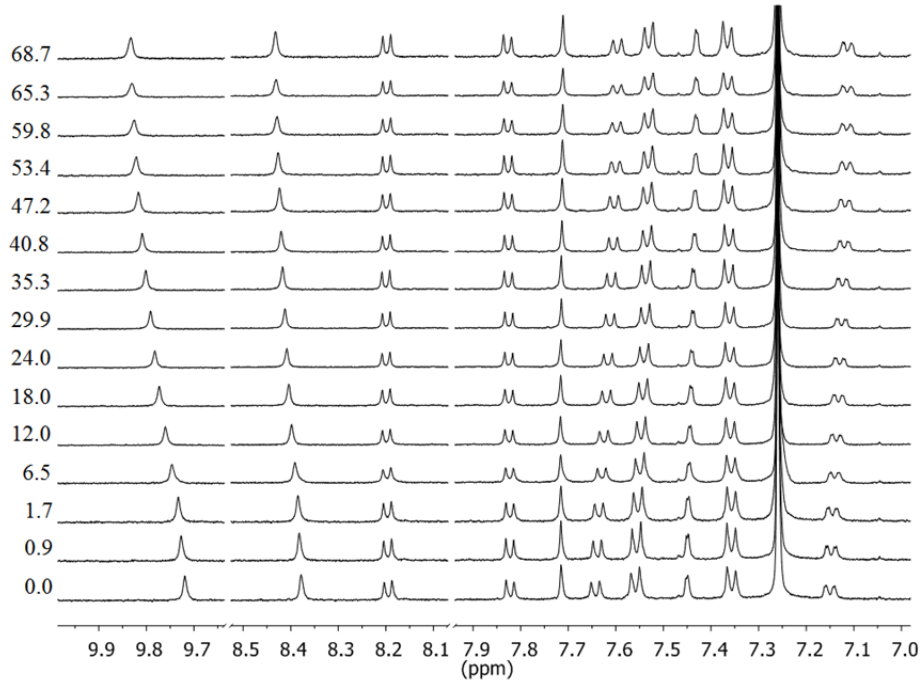

Fig. S26 Representative stacked ^{1}H NMR titration data for **2**·I^{-}. [Guest]/[Host] listed on left.

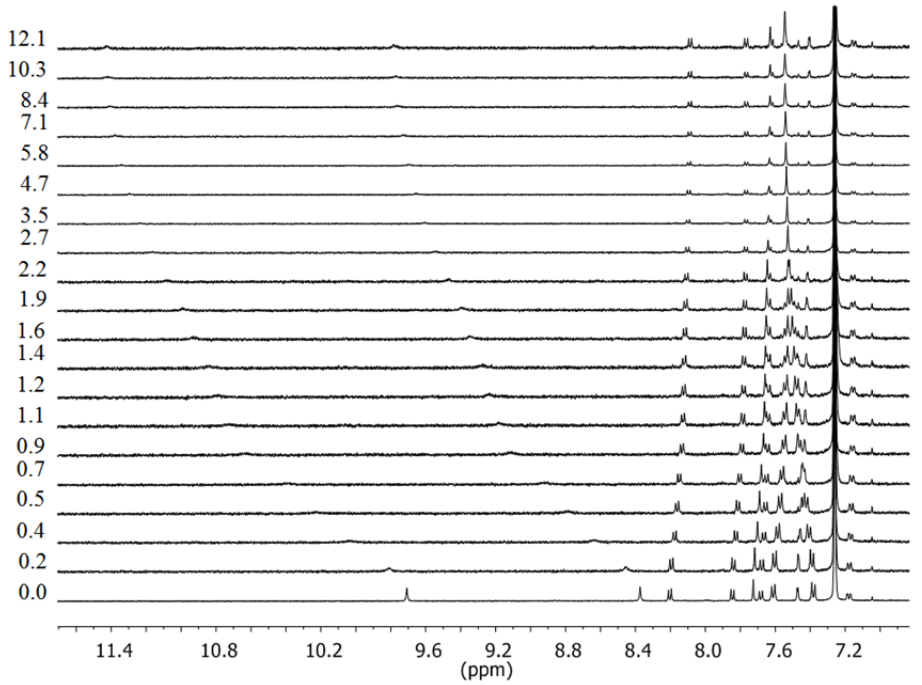

Fig. S27 Representative stacked ^{1}H NMR titration data for **2**·OAc^{-}. [Guest]/[Host] listed on left.

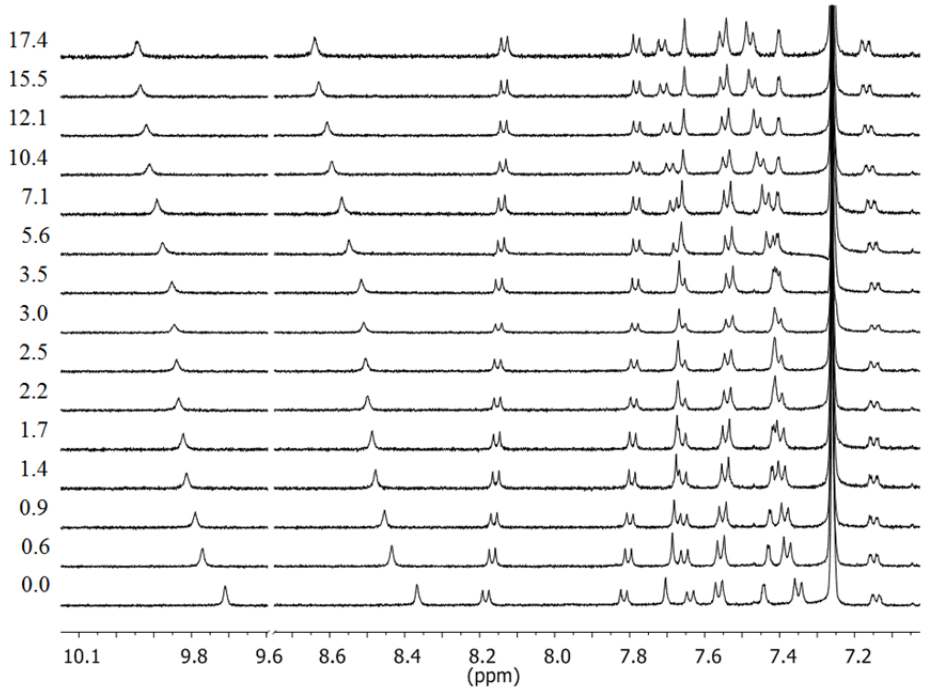

Fig. S28 Representative stacked ^{1}H NMR titration data for **2**·HSO_4^-. [Guest]/[Host] listed on left.

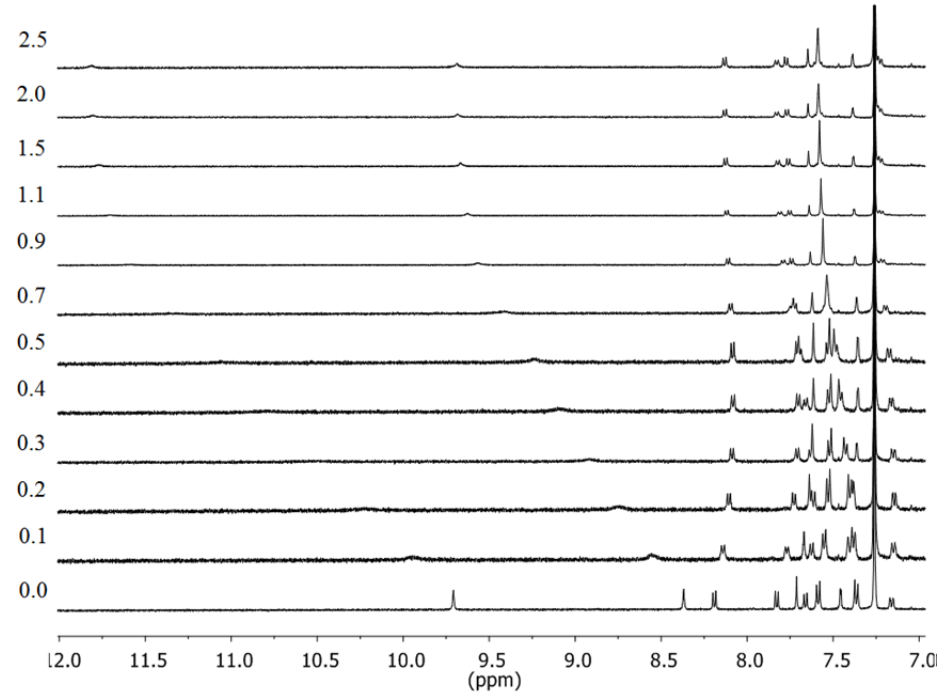

Fig. S29 Representative stacked ^{1}H NMR titration data for **2**·$H_2PO_4^-$. [Guest]/[Host] listed on left.

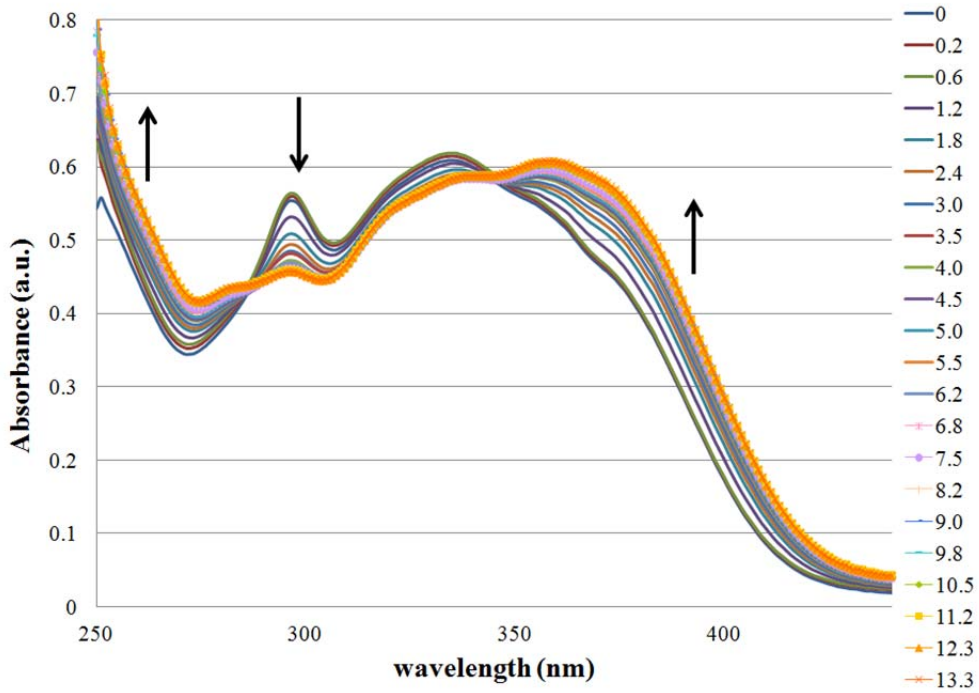

Fig. S30 Representative UV/Vis titration spectra for **2**·$H_2PO_4^-$. [Guest]/[Host] in legend.

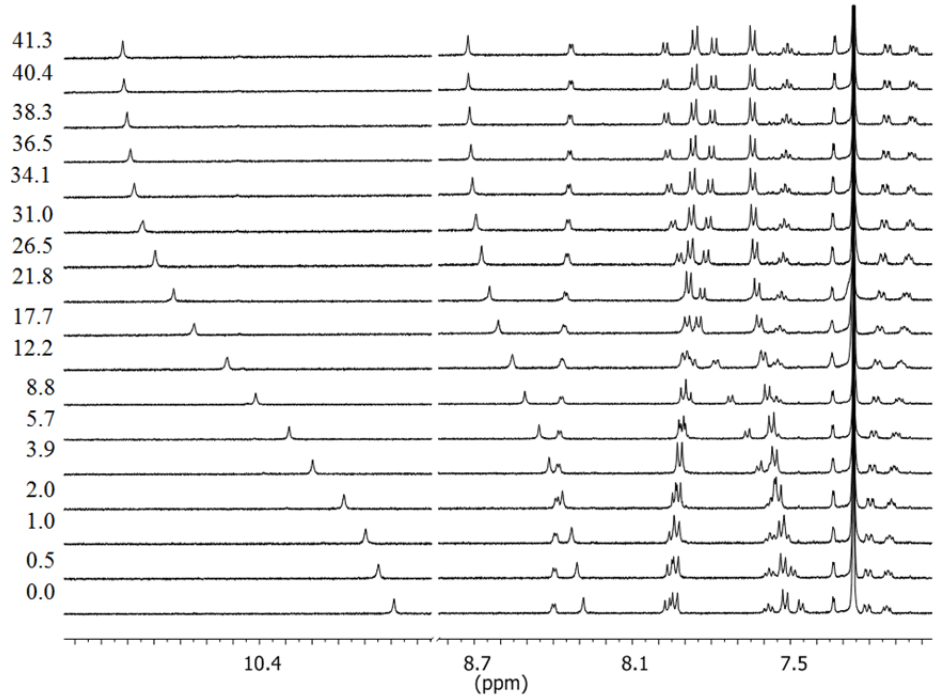

Fig. S31 Representative stacked ^{1}H NMR titration data for **3**·Cl^-. [Guest]/[Host] listed on left.

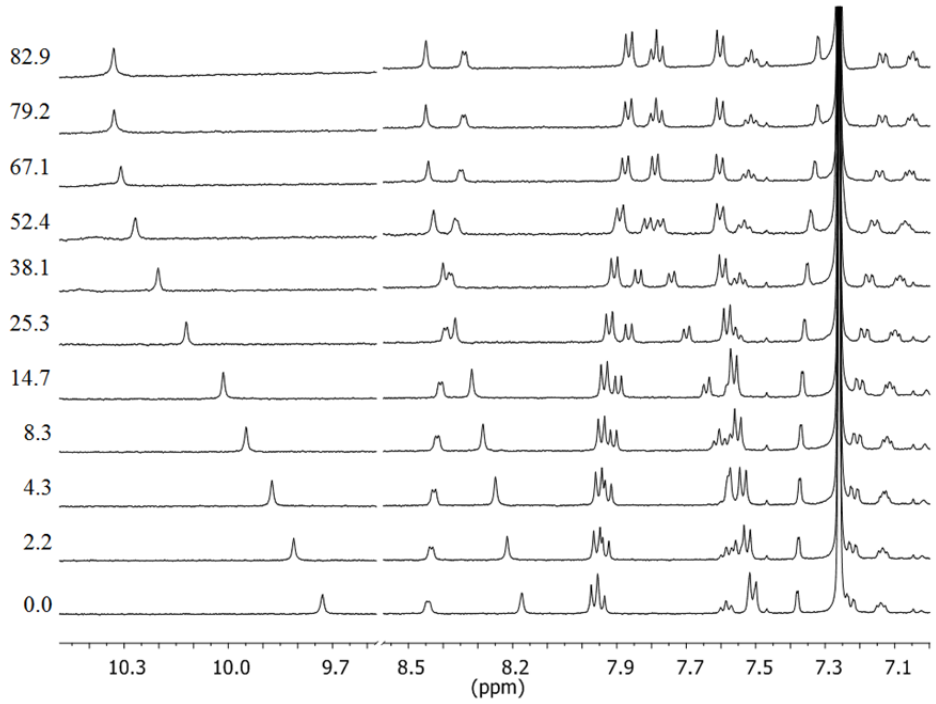

Fig. S32 Representative stacked ^{1}H NMR titration data for **3**·Br^{-}. [Guest]/[Host] listed on left.

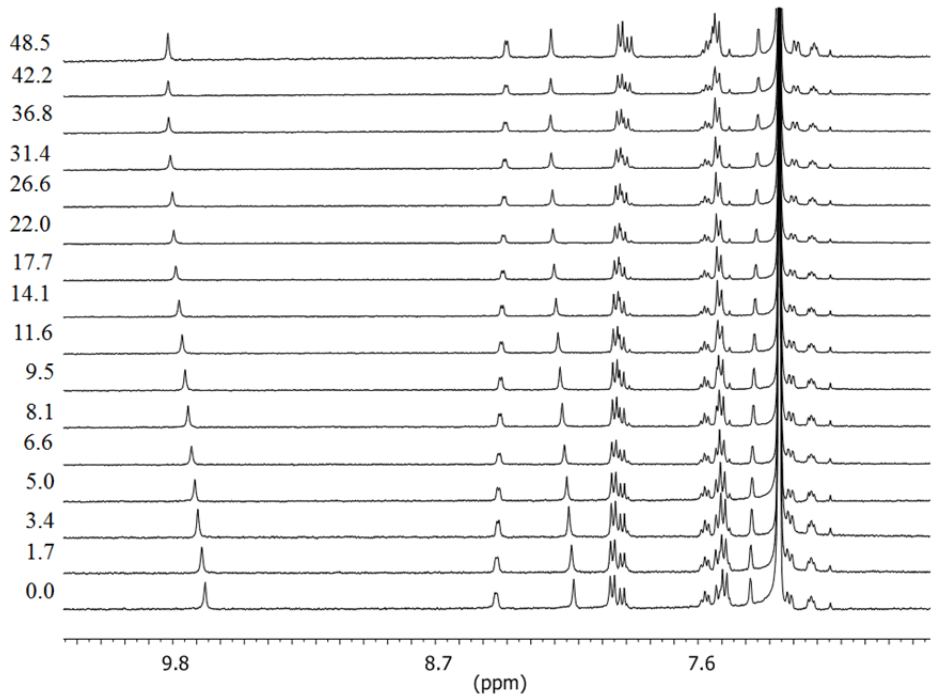

Fig. S33 Representative stacked ^{1}H NMR titration data for **3**·I^{-}. [Guest]/[Host] listed on left.

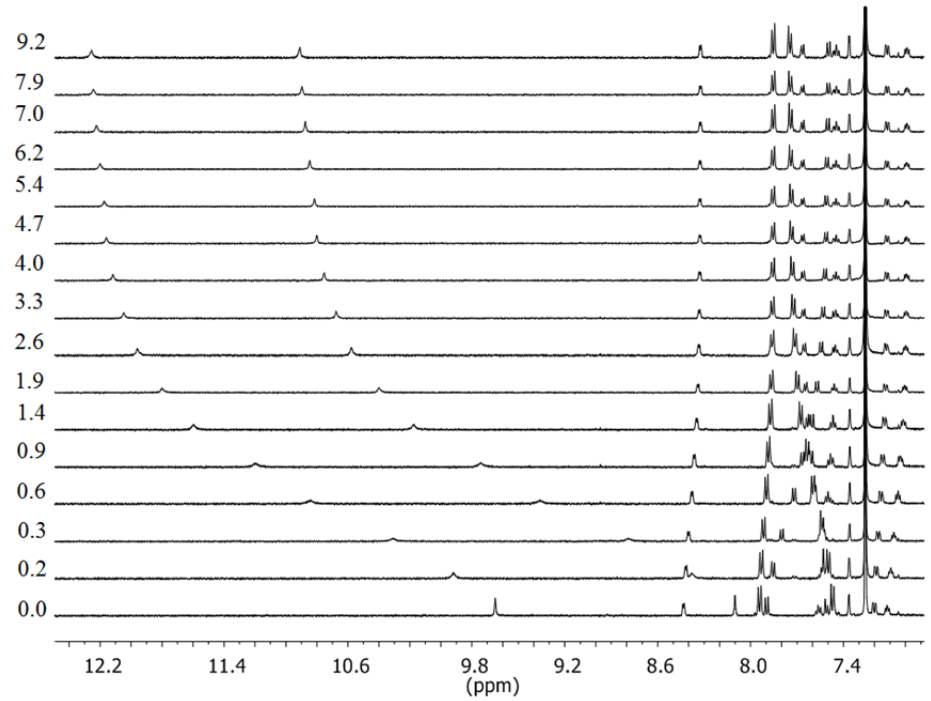

Fig. S34 Representative stacked ^{1}H NMR titration data for **3**·OAc^{-}. [Guest]/[Host] listed on left.

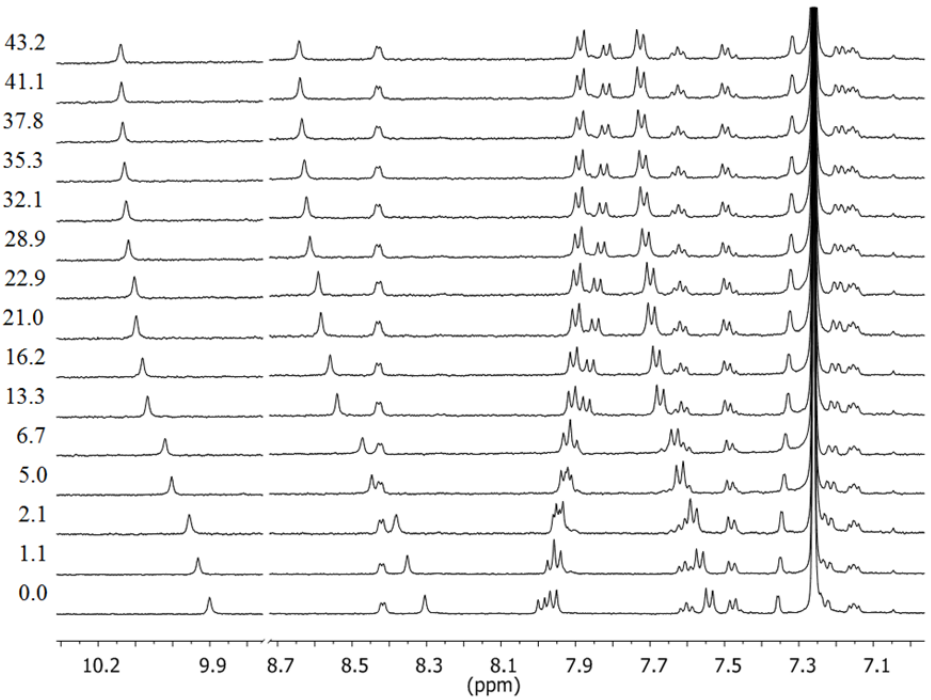

Fig. S 35 Representative stacked ^{1}H NMR titration data for **3**·HSO_4^-. [Guest]/[Host] listed on left.

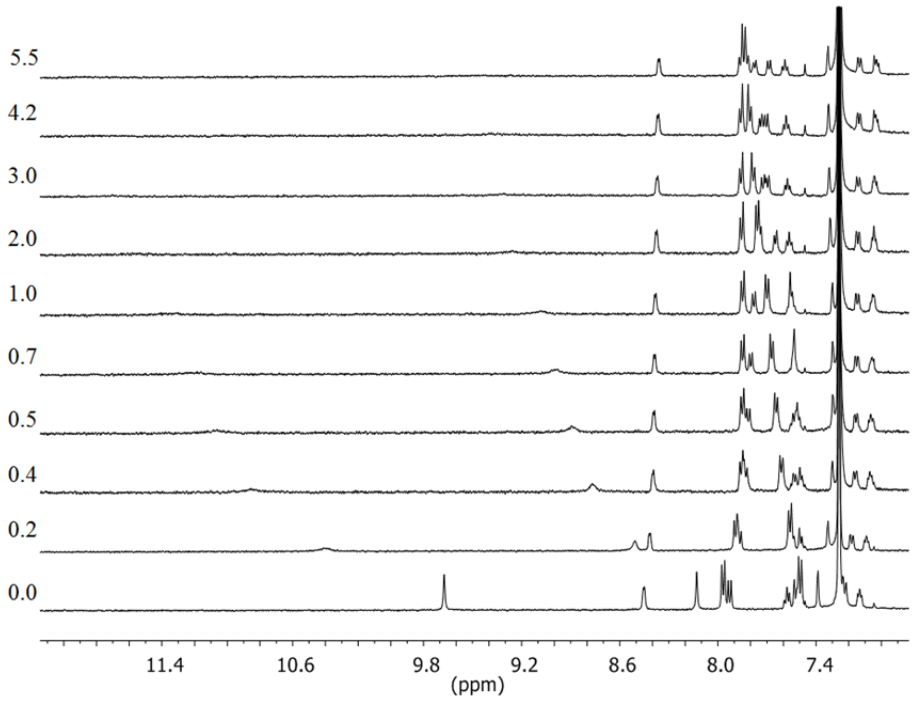

Fig. S36 Representative stacked ^{1}H NMR titration data for **3**·$H_2PO_4^-$. [Guest]/[Host] listed on left.

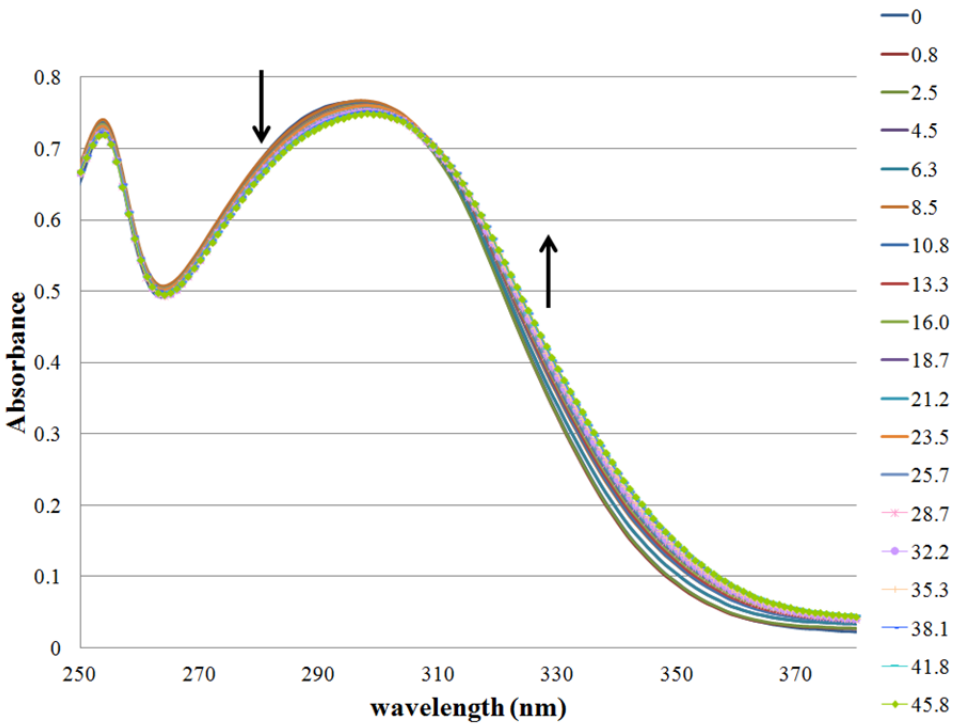

Fig. S37 Representative UV/Vis titration spectra for **3**·$H_2PO_4^-$. [Guest]/[Host] in legend.

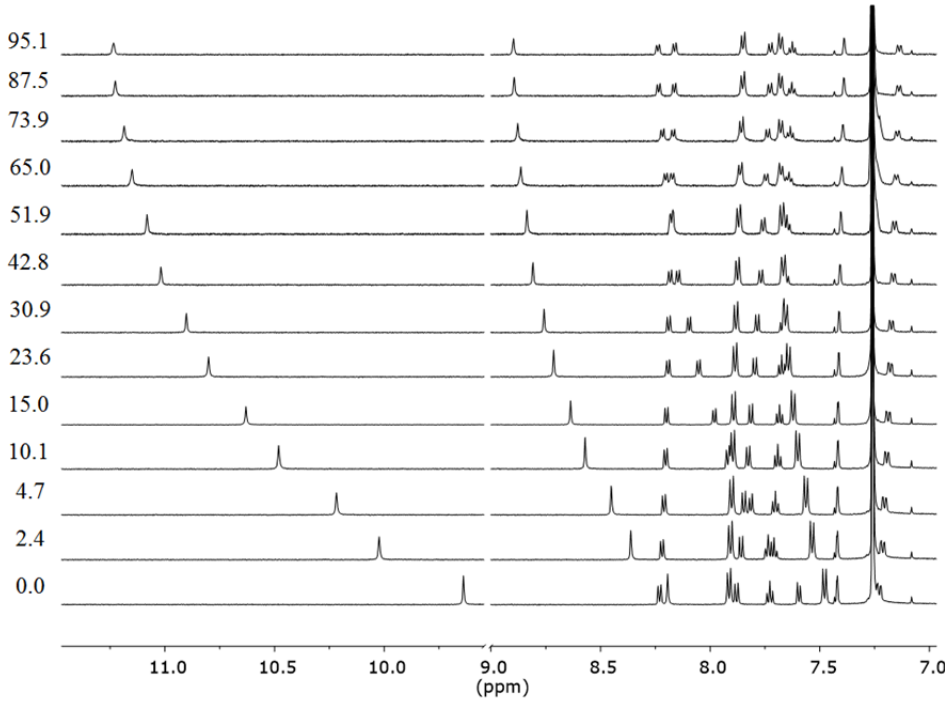

Fig. S 38 Representative stacked ^{1}H NMR titration data for **1**·Cl^{-}. [Guest]/[Host] listed on left.

Job's Plot Analysis

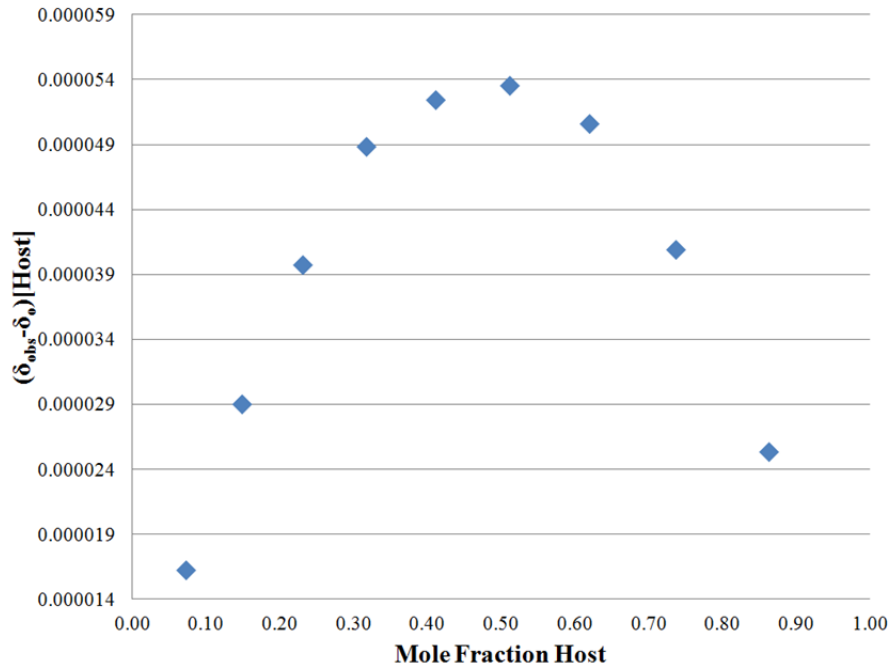

Fig. S39 Job's Plot for **2**·Cl^{-}.

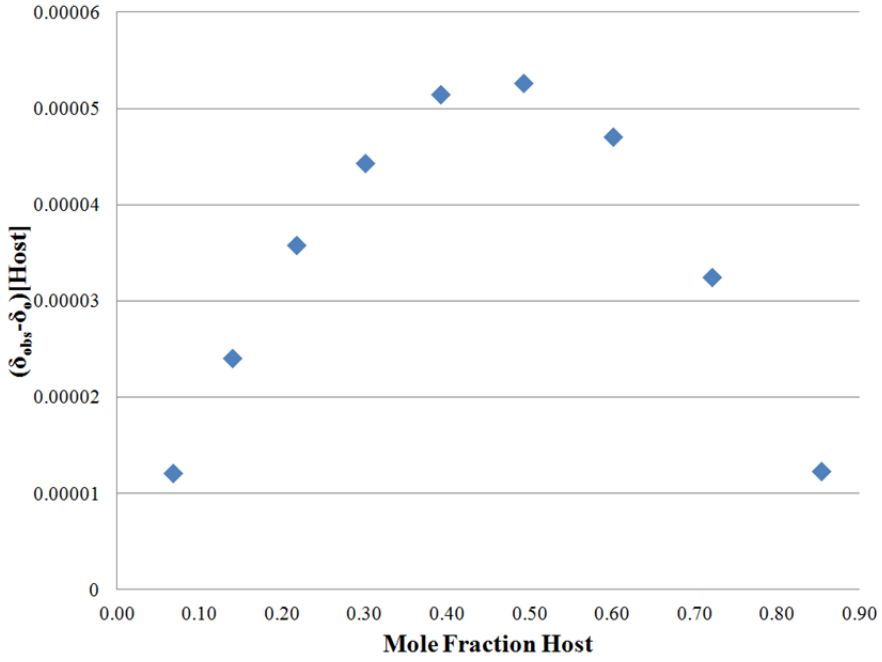

Fig. S40 Job's Plot for **2**·OAc^-.

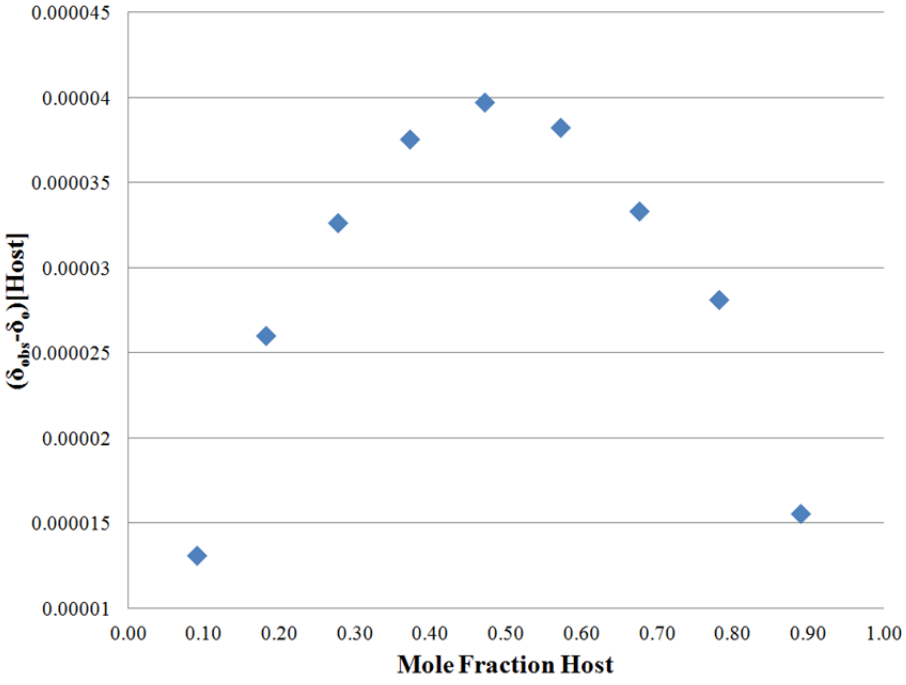

Fig. S41 Job's Plot for **2**·HSO_4^-.

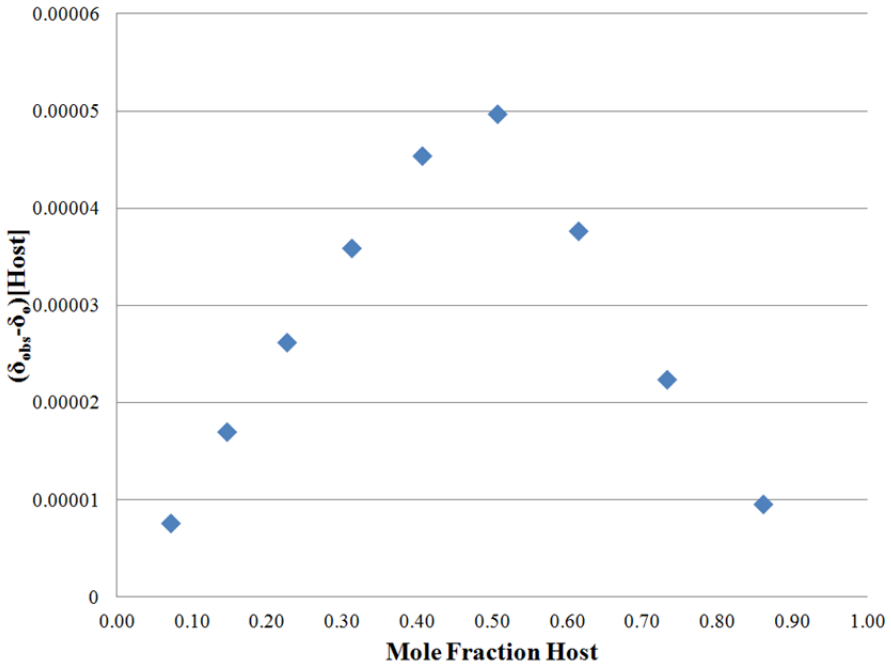

Fig. S42 Job's Plot for **2**·$H_2PO_4^-$.

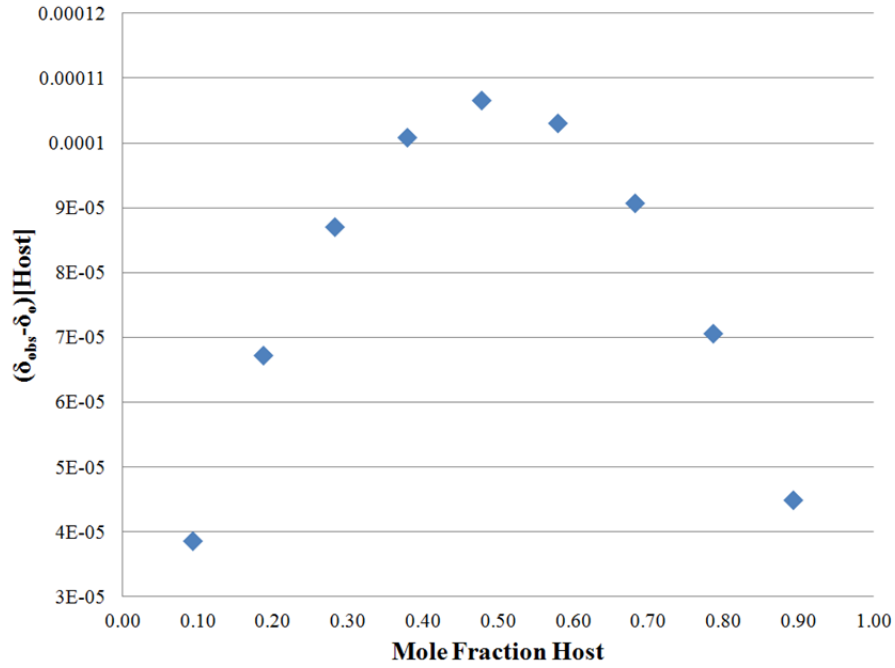

Fig. S43 Job's Plot for **3**·Cl^-.

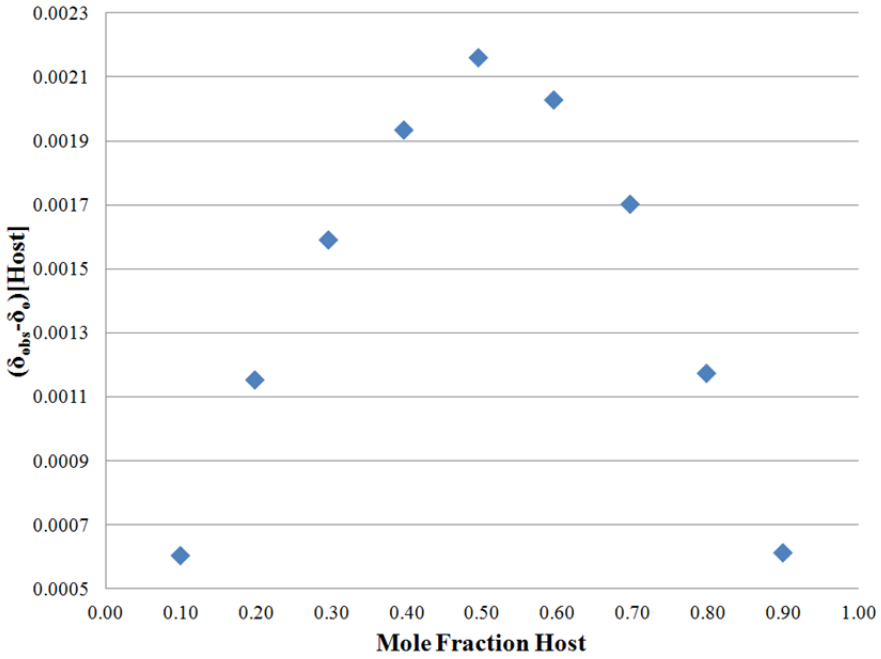

Fig. S44 Job's Plot for **3**·OAc^-.

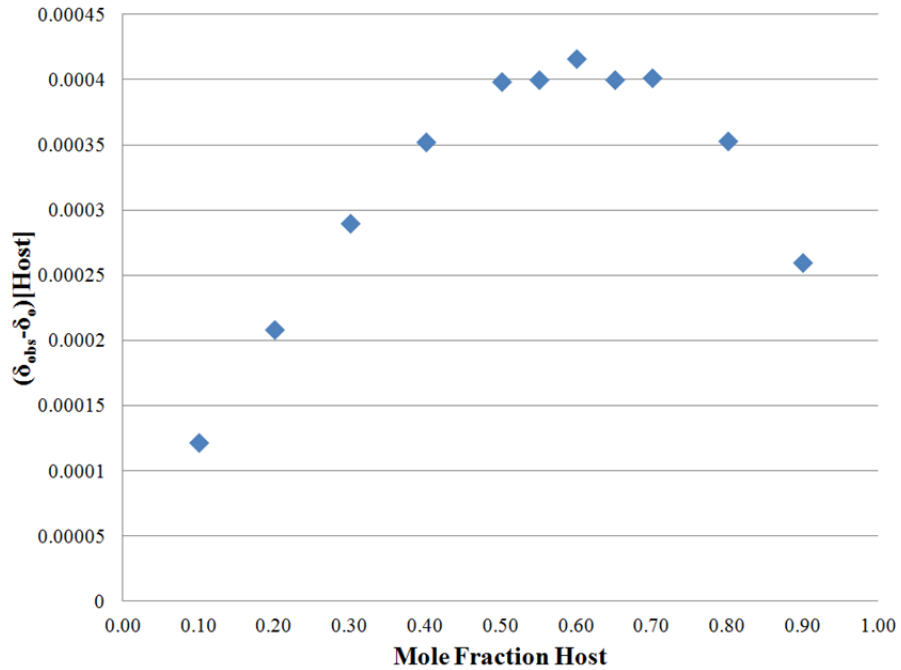

Fig. S45 Job's Plot for **3**·HSO_4^-.

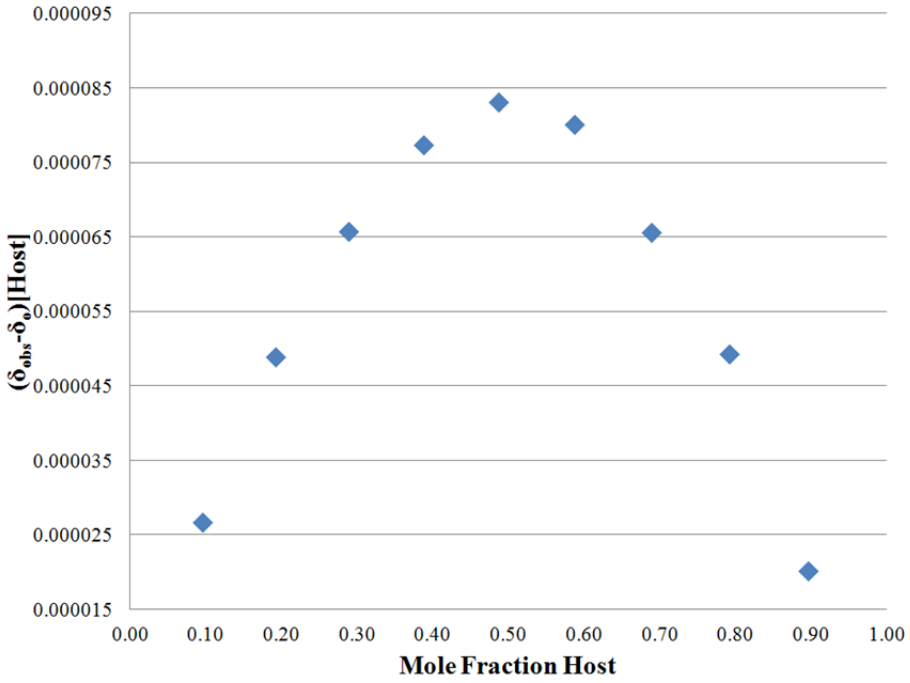

Fig. S46 Job's Plot for **3**·$H_2PO_4^-$.

Representative Revised Fit Binding Curves of 1

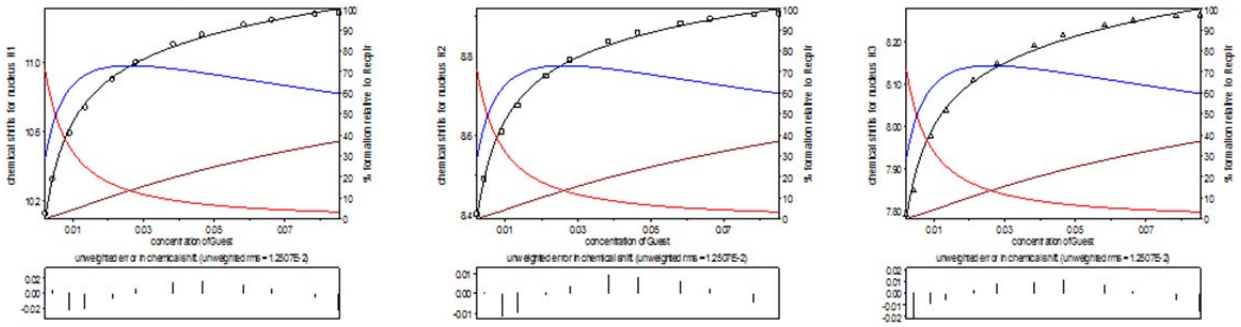

Fig. S47 Representative revised fit of titration data of **1**·Cl^-. β_{12} held constant at 1590 M^{-1}.

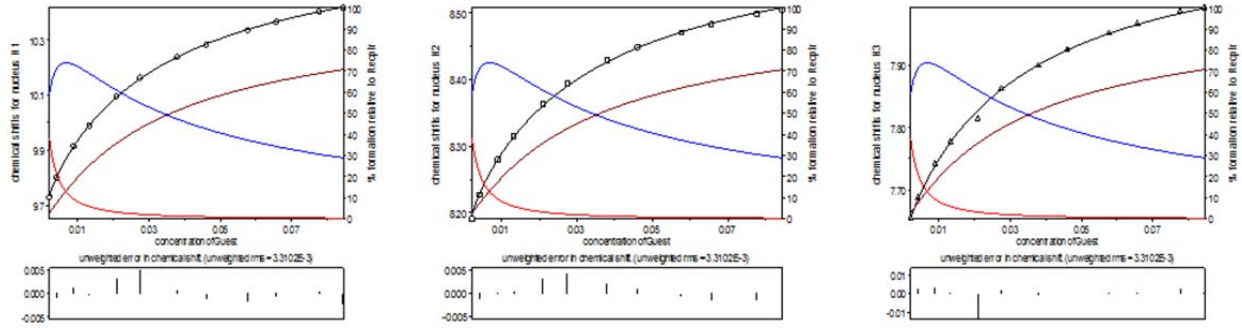

Fig. S48 Representative revised fit of titration data of **1**·Br^-. β_{12} held constant at 1590 M^{-1}.

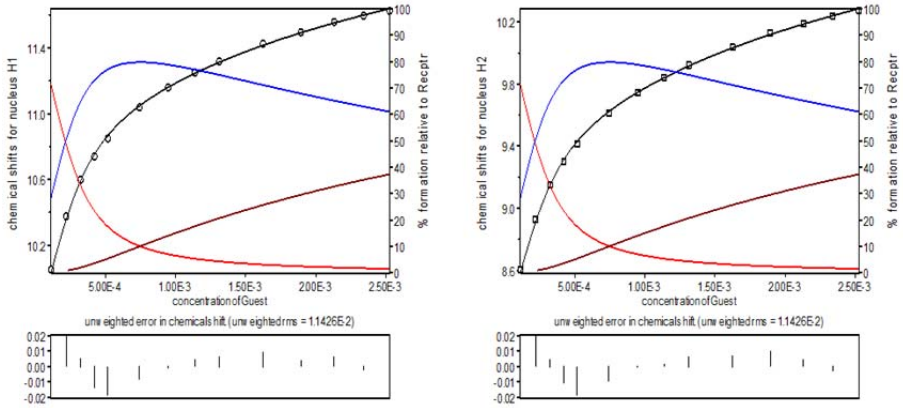

Fig. S49 Representative revised fit of titration data of **1**·OAc^-. β_{12} held constant at 5,250,000 M^{-1}.

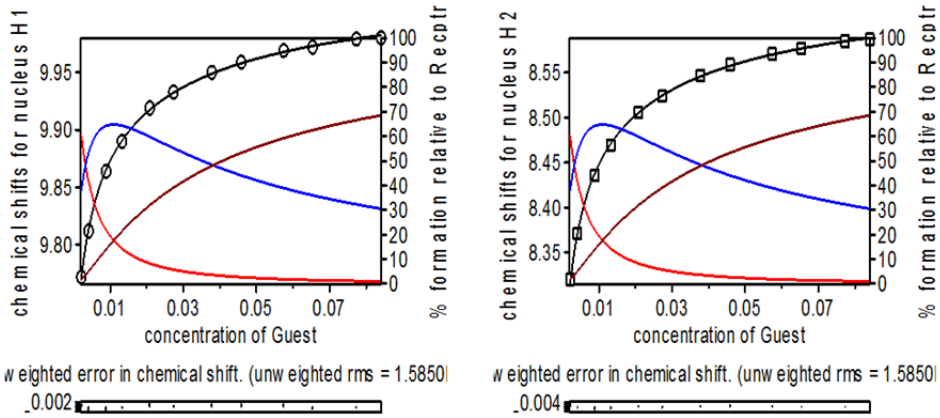

Fig. S50 Representative revised fit of titration data of **1**·HSO_4^-. β_{12} held constant at 10,000 M^{-1}.

Cartesian Coordinates of DFT Structures

Structures were minimized using the ωB97X-D method and 6-31G(d,p) basis set. All energies are given in Hartrees.

2·Cl^- **W** conformation

Energy = -3279.35275931

Sum of electronic and zero-point Energies = -3278.508925

Imaginary Frequencies = 0

Atom	X	Y	Z
H	-6.08481	-0.23589	-0.80297
H	-7.80631	-1.28488	-0.31463
H	7.679908	-1.16435	0.8322
H	5.873902	-0.31617	1.270413
H	4.142681	-3.56024	1.154883
H	3.003051	-5.76509	0.778628
H	-1.4521	-6.99372	-0.4664
H	0.92247	-7.01639	0.181283
H	-3.52325	-5.69932	-1.00666
H	-4.63851	-3.48246	-1.2873
H	-7.03394	3.353277	-1.01917
H	-5.36221	5.083301	-1.40207
H	-2.28237	2.098535	-1.51017
H	-1.20606	3.676229	-2.86089
H	-0.86634	3.732308	-1.11876
H	-0.53687	5.140013	-2.12618
H	-4.0232	6.19818	-2.78931
H	-3.0993	5.109264	-3.83752
H	-2.31225	6.513885	-3.09416
H	-2.31121	5.166666	0.421866
H	-3.56984	6.215086	-0.25506
H	-1.86375	6.557034	-0.58441
H	-9.27333	-2.88572	0.189143
H	-11.5873	-3.56874	0.704635
H	-12.8742	0.506206	0.35676
H	-10.5564	1.207896	-0.16374
H	6.576926	3.27204	1.443396
H	4.881835	4.966333	1.847816
H	1.825262	1.966442	1.589087
H	0.626871	3.674234	0.698909
H	1.622176	4.881288	-0.12847
H	0.321245	5.39421	0.962064
H	0.547989	5.039056	3.479396

H	0.865192	3.318061	3.221338
H	2.015022	4.297382	4.147438
H	1.84095	6.784046	2.310967
H	3.346015	6.157111	2.99128
H	3.190954	6.397477	1.238442
H	9.624971	1.450657	-0.99483
H	11.85758	0.942163	-1.94821
H	11.60712	-3.06802	-0.45246
H	9.373232	-2.57225	0.501183
C	2.346897	-2.44231	0.686949
C	3.098916	-3.62708	0.860123
C	2.46798	-4.82885	0.652
C	1.108856	-4.8522	0.274672
C	0.454111	-3.60956	0.120094
C	-0.94971	-3.59585	-0.27544
C	-1.61762	-4.82555	-0.4762
C	-0.9143	-6.06507	-0.30342
C	0.393419	-6.07721	0.053141
C	-2.97748	-4.77478	-0.84635
C	-3.59569	-3.55863	-1.00296
C	-2.83382	-2.38832	-0.78698
C	-3.4169	-1.08527	-0.94817
C	-3.82229	0.050672	-1.06443
C	-4.26425	1.404214	-1.1776
C	-5.62733	1.73309	-1.03634
C	-5.99546	3.078391	-1.12781
C	-5.02967	4.050968	-1.34745
C	-3.66919	3.750451	-1.49729
C	-3.3148	2.409703	-1.40762
C	-2.64219	4.867614	-1.71557
C	-1.23482	4.311969	-1.96989
C	-3.04945	5.720883	-2.93116
C	-2.59799	5.754286	-0.45631
C	-7.86709	0.757541	-0.54877
C	-9.75548	-0.78816	-0.02441
C	-10.0597	-2.13878	0.223615
C	-11.3517	-2.52999	0.513574
C	-12.3533	-1.56447	0.558645
C	-12.0765	-0.22436	0.316483
C	-10.781	0.169588	0.024264
C	2.944748	-1.15558	0.910766
C	3.388631	-0.04457	1.098123

C	3.826815	1.297947	1.314949
C	5.192832	1.646812	1.266576
C	5.536076	2.98305	1.473228
C	4.555998	3.943248	1.699646
C	3.196546	3.623432	1.749554
C	2.862964	2.28352	1.560058
C	2.093554	4.660657	1.995766
C	1.109996	4.649312	0.810668
C	1.33625	4.303111	3.288773
C	2.66037	6.079073	2.141514
C	7.365321	0.830251	0.436875
C	9.348723	-0.52514	-0.18168
C	10.05813	0.469131	-0.87894
C	11.30437	0.1836	-1.40919
C	11.8504	-1.0858	-1.25023
C	11.16402	-2.08705	-0.56544
C	9.921298	-1.80474	-0.03624
N	1.068146	-2.43044	0.326138
N	-1.55401	-2.40433	-0.43278
N	-6.51998	0.677623	-0.80899
N	-8.42634	-0.48842	-0.31143
N	-13.7147	-1.96706	0.865666
N	8.09616	-0.33963	0.379893
N	6.144417	0.641126	1.047788
N	13.15729	-1.37265	-1.80734
O	-8.504	1.799916	-0.52904
O	-13.9362	-3.15557	1.06793
O	-14.581	-1.10132	0.909417
O	7.750889	1.907681	0.000574
O	13.62196	-2.49767	-1.65378
O	13.74446	-0.47899	-2.40864
Cl	6.54444	-2.67588	1.844284

2·Cl^- **U** conformation

Energy = -3279.382261

Sum of electronic and zero-point Energies = -3287.537348

Imaginary Frequencies = 0

Atom	X	Y	Z
H	-2.10123	-0.25691	-1.7077
H	-0.26706	-1.1413	-1.98677
H	0.395091	0.048614	0.234895

H	2.322596	0.583918	-0.11955
H	4.383242	5.747022	0.453714
H	2.933918	7.77013	0.61376
H	-1.79405	8.457922	0.408661
H	0.645845	8.756376	0.610612
H	-3.75032	6.959745	0.057437
H	-4.62625	4.659243	-0.34029
H	-4.5013	-3.03161	-1.86583
H	-6.86477	-2.80795	-1.34723
H	-6.24531	1.30636	-0.31021
H	-8.47003	1.523001	-0.73777
H	-8.12667	1.062712	0.94356
H	-9.73179	0.789912	0.257603
H	-8.884	-2.00124	-2.03595
H	-8.86585	-0.29207	-2.50053
H	-10.1582	-0.91898	-1.46022
H	-8.01062	-1.40459	1.596959
H	-8.36971	-2.66344	0.405483
H	-9.65408	-1.57623	0.949468
H	1.884655	-1.54406	-2.30212
H	3.881047	-2.91452	-1.78937
H	1.364184	-5.93288	-0.07165
H	-0.64344	-4.56823	-0.58897
H	4.353903	-2.34731	0.664309
H	6.775485	-2.35808	0.469609
H	6.75393	1.892147	-0.14214
H	8.458523	1.307377	-1.6167
H	8.441608	-0.36332	-2.20384
H	9.941333	0.343604	-1.57264
H	10.20457	0.780486	0.91232
H	8.73866	1.76697	0.912408
H	8.883867	0.405547	2.036022
H	10.22291	-1.51535	0.034949
H	8.941621	-1.9988	1.152707
H	8.771819	-2.30594	-0.58824
H	0.451229	-3.12721	2.094789
H	-1.65822	-4.1899	2.860966
H	-3.86096	-0.69655	1.708832
H	-1.7648	0.375246	0.949435
C	2.68727	4.413607	0.219658
C	3.304151	5.674253	0.389992
C	2.501389	6.783796	0.477847

C	1.101231	6.643239	0.388247
C	0.584261	5.338966	0.209524
C	-0.85921	5.161334	0.084386
C	-1.69067	6.302953	0.153985
C	-1.12368	7.60583	0.355129
C	0.216409	7.770121	0.465766
C	-3.07926	6.107912	0.007323
C	-3.56687	4.844898	-0.20971
C	-2.64905	3.767769	-0.26824
C	-3.16814	2.449773	-0.51419
C	-3.72219	1.393474	-0.73364
C	-4.52108	0.223166	-0.93088
C	-3.99518	-1.00806	-1.36624
C	-4.88029	-2.08148	-1.52042
C	-6.22395	-1.94087	-1.21865
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C	-5.8942	0.337876	-0.64578
C	-8.26174	-0.63624	-0.43176
C	-8.66097	0.770265	0.033909
C	-9.08837	-0.98597	-1.68376
C	-8.58993	-1.63225	0.696826
C	-1.89768	-2.28914	-1.4822
C	0.487657	-2.96347	-1.4741
C	1.774058	-2.51256	-1.82659
C	2.890214	-3.26816	-1.53627
C	2.72635	-4.49418	-0.89532
C	1.463556	-4.97476	-0.56554
C	0.341629	-4.21578	-0.85434
C	3.483651	3.221111	0.1468
C	4.145716	2.207027	0.11784
C	4.858381	0.969493	0.152475
C	4.150094	-0.23457	0.361619
C	4.874686	-1.41736	0.485468
C	6.261809	-1.40861	0.37479
C	6.983259	-0.23679	0.131766
C	6.250485	0.946016	0.028832
C	8.508313	-0.20443	-0.02734
C	8.854968	0.303182	-1.44026
C	9.115586	0.746015	1.021933
C	9.13816	-1.5915	0.155843
C	1.923182	-1.0121	1.107289
C	-0.51756	-1.31211	1.459653

C	-0.48742	-2.59954	2.019385
C	-1.66469	-3.19018	2.445942
C	-2.86686	-2.5021	2.319928
C	-2.91474	-1.21502	1.793398
C	-1.74005	-0.62382	1.373078
N	1.372374	4.251515	0.135004
N	-1.34047	3.918043	-0.11178
N	-2.62902	-1.12448	-1.65221
N	-0.5595	-2.09577	-1.74679
N	3.898183	-5.27199	-0.5473
N	0.596172	-0.67049	0.932321
N	2.751877	-0.17945	0.392853
N	-4.10134	-3.14279	2.731332
O	-2.38576	-3.36301	-1.16072
O	5.00443	-4.77354	-0.73584
O	3.737753	-6.39142	-0.07324
O	2.316322	-1.92024	1.826739
O	-5.1556	-2.53913	2.561562
O	-4.03951	-4.2628	3.227203
Cl	0.300182	0.90781	-1.92132

2·OAc$^-$ **W** conformation

Energy = -3047.562228

Sum of electronic and zero-point Energies = -3046.667425

Imaginary Frequencies = 0

Atom	X	Y	Z
H	-6.47316	-0.17337	-0.13641
H	-8.11902	-1.42082	0.02644
H	7.981086	-0.67957	-0.79065
H	5.932754	-0.07024	-0.59916
H	4.079104	-3.09139	-0.91287
H	2.908978	-5.32745	-1.09112
H	-1.69965	-6.61977	-1.04929
H	0.760065	-6.60492	-1.13104
H	-3.85465	-5.36188	-0.86554
H	-5.03011	-3.17004	-0.64676
H	-7.74081	3.306257	0.183935
H	-6.24748	5.220128	-0.01417
H	-2.91554	2.579428	-0.59262
H	-1.96408	4.382214	-1.65144
H	-1.65538	4.322963	0.097333

H	-1.47674	5.840338	-0.7837
H	-5.0575	6.53867	-1.44172
H	-3.99594	5.650834	-2.54742
H	-3.39339	7.080768	-1.68821
H	-3.25413	5.490799	1.717282
H	-4.61521	6.44261	1.100514
H	-2.95728	6.987956	0.813195
H	-9.46028	-3.19673	0.13462
H	-11.6766	-4.16689	0.620306
H	-13.1641	-0.27469	1.630177
H	-10.946	0.715087	1.141386
H	6.739729	3.456223	0.081837
H	5.147048	5.282614	0.024099
H	1.954433	2.475142	-0.53654
H	1.077009	4.174823	-1.78197
H	2.301063	5.250036	-2.47829
H	0.862589	5.926468	-1.68953
H	0.588984	5.756905	0.835211
H	0.826461	4.006561	0.768042
H	1.851684	4.99452	1.821954
H	2.2082	7.320641	-0.18157
H	3.507589	6.659217	0.815526
H	3.702056	6.766512	-0.94631
H	9.492491	0.875952	2.276865
H	11.61344	-0.00236	3.213282
H	11.78587	-2.95754	0.111567
H	9.651554	-2.09369	-0.82458
H	7.077461	-3.68989	-3.51703
H	6.26121	-4.31371	-2.0635
H	5.345008	-3.36064	-3.22685
C	2.213341	-2.0302	-0.73015
C	2.998285	-3.19849	-0.87707
C	2.349549	-4.40343	-0.97821
C	0.939221	-4.44705	-0.93611
C	0.253016	-3.21945	-0.79806
C	-1.20489	-3.22752	-0.76039
C	-1.88739	-4.46274	-0.84919
C	-1.14946	-5.68643	-0.98246
C	0.20543	-5.67745	-1.02708
C	-3.29679	-4.43272	-0.80322
C	-3.94869	-3.23053	-0.68306
C	-3.17105	-2.05256	-0.60996

C	-3.7981	-0.76575	-0.49786
C	-4.26414	0.349583	-0.41278
C	-4.81454	1.662477	-0.30704
C	-6.19546	1.841921	-0.08683
C	-6.68677	3.146322	0.013048
C	-5.8214	4.225119	-0.10215
C	-4.4457	4.075123	-0.32391
C	-3.96748	2.774242	-0.4226
C	-3.54066	5.306779	-0.43928
C	-2.07805	4.929296	-0.70996
C	-4.03092	6.195044	-1.59843
C	-3.59924	6.103105	0.878178
C	-8.31848	0.604096	0.323583
C	-10.052	-1.17017	0.602226
C	-10.2701	-2.55223	0.460827
C	-11.5063	-3.10412	0.731675
C	-12.5385	-2.26928	1.150655
C	-12.3452	-0.9013	1.300837
C	-11.1057	-0.34598	1.028681
C	2.850649	-0.75122	-0.60355
C	3.381156	0.330905	-0.48973
C	3.908834	1.650751	-0.35778
C	5.287665	1.90055	-0.1811
C	5.690343	3.233699	-0.05333
C	4.768243	4.272462	-0.08347
C	3.399326	4.047082	-0.25697
C	3.002773	2.720122	-0.39654
C	2.352734	5.167471	-0.29684
C	1.605052	5.122922	-1.64306
C	1.345941	4.96582	0.851673
C	2.989049	6.555153	-0.14293
C	7.414298	0.874514	0.472347
C	9.425625	-0.55385	0.664233
C	9.988287	0.037586	1.811683
C	11.17513	-0.45082	2.330603
C	11.81272	-1.52366	1.714795
C	11.27589	-2.12283	0.575288
C	10.09215	-1.64127	0.057969
C	6.670604	-2.20448	-1.97523
C	6.326576	-3.46933	-2.75724
N	0.884954	-2.03516	-0.69593
N	-1.84386	-2.04916	-0.64324

N	-6.98464	0.688397	0.003484
N	-8.77302	-0.70543	0.308325
N	-13.843	-2.84096	1.435614
N	8.23586	-0.1628	0.079089
N	6.203678	0.84295	-0.19002
N	13.05277	-2.02628	2.265285
O	-9.0264	1.563688	0.589023
O	-13.9909	-4.04928	1.29186
O	-14.7377	-2.0903	1.807106
O	7.722435	1.721677	1.305268
O	13.60065	-2.97097	1.704322
O	13.50728	-1.48895	3.27116
O	5.815897	-1.79605	-1.14411
O	7.783921	-1.65142	-2.19114

2·OAc^- **U** conformation

Energy = -3047.592132

Sum of electronic and zero-point Energies = -3046.695303

Imaginary Frequencies = 0

Atom	X	Y	Z
H	-2.53947	-0.96556	-0.42914
H	-0.70806	-1.72993	-0.32768
H	1.306744	-0.6037	2.419108
H	2.352585	0.698587	1.33863
H	2.634888	5.868311	1.956683
H	0.897708	7.358946	2.948797
H	-3.87668	7.083185	3.259528
H	-1.52482	7.794644	3.428722
H	-5.57198	5.413241	2.489854
H	-6.06357	3.273075	1.305495
H	-3.99986	-3.20863	-2.88249
H	-6.36931	-3.28849	-3.43667
H	-7.02198	0.285057	-1.1533
H	-8.88545	0.514587	-2.42852
H	-9.14995	-0.4702	-0.97361
H	-10.27	-0.5797	-2.33529
H	-8.04795	-2.36687	-4.71764
H	-8.17522	-0.60318	-4.61767
H	-9.62943	-1.61162	-4.48508
H	-8.83842	-3.01511	-1.08049
H	-8.45333	-3.79909	-2.62067

H	-10.0262	-3.02406	-2.39795
H	1.381215	-2.53865	0.242825
H	3.762393	-2.71201	-0.38673
H	2.734405	-1.89903	-4.47658
H	0.332409	-1.79369	-3.86005
H	5.395649	-1.13141	0.273357
H	6.735708	-0.42347	-1.61079
H	4.516485	3.240982	-1.82064
H	4.698314	2.735087	-4.13554
H	4.980799	1.023955	-4.50216
H	5.983356	2.276555	-5.26353
H	7.679215	3.567219	-3.86389
H	6.423867	4.030986	-2.71022
H	7.88143	3.201757	-2.14034
H	8.067603	1.209557	-4.48101
H	8.319102	0.758158	-2.79031
H	7.127149	-0.11464	-3.77929
H	3.687926	-3.23369	3.603959
H	2.864184	-5.27667	4.744946
H	-1.18742	-4.02173	4.112882
H	-0.37161	-1.9852	2.93518
H	0.613899	0.932584	-0.88539
H	-1.15569	0.796658	-1.07008
H	-0.43692	2.161067	-0.15829
C	1.166706	4.441157	1.241078
C	1.580808	5.625715	1.892917
C	0.620479	6.440886	2.440084
C	-0.73918	6.077116	2.350791
C	-1.0468	4.87448	1.675733
C	-2.43821	4.451227	1.575527
C	-3.43856	5.262023	2.157143
C	-3.0837	6.481628	2.826375
C	-1.78951	6.873409	2.919392
C	-4.77396	4.820176	2.05403
C	-5.05026	3.643879	1.404421
C	-3.97415	2.9082	0.851127
C	-4.25323	1.689409	0.144619
C	-4.55884	0.691552	-0.47139
C	-5.01547	-0.42576	-1.23667
C	-4.13714	-1.41778	-1.70735
C	-4.66144	-2.44039	-2.50544
C	-6.01055	-2.47333	-2.81526

C	-6.91235	-1.50998	-2.33813
C	-6.38514	-0.49742	-1.54821
C	-8.40118	-1.60533	-2.69004
C	-9.21584	-0.46427	-2.06634
C	-8.5691	-1.54376	-4.21986
C	-8.95918	-2.94232	-2.16591
C	-1.75049	-1.90755	-2.06933
C	0.699819	-2.14162	-1.76445
C	1.680804	-2.40566	-0.79201
C	3.012998	-2.50647	-1.13961
C	3.375439	-2.31027	-2.47008
C	2.422942	-2.04854	-3.45048
C	1.083617	-1.98049	-3.1061
C	2.138809	3.542653	0.678008
C	2.956743	2.775962	0.221172
C	3.939368	1.873273	-0.2959
C	4.133134	0.599385	0.289013
C	5.190174	-0.17778	-0.18687
C	5.957827	0.246958	-1.26526
C	5.726166	1.457846	-1.91668
C	4.723808	2.268868	-1.38437
C	6.481832	1.886705	-3.17852
C	5.472071	1.988502	-4.33869
C	7.153251	3.253622	-2.956
C	7.56113	0.868903	-3.57277
C	3.263148	-1.03009	1.941139
C	1.711197	-2.46483	3.219897
C	2.628296	-3.40427	3.720925
C	2.167484	-4.54648	4.35342
C	0.798599	-4.75227	4.493824
C	-0.1273	-3.83365	4.002031
C	0.329041	-2.69701	3.365102
C	-0.37491	0.321243	0.906342
C	-0.35254	1.098647	-0.39627
N	-0.10572	4.088058	1.126989
N	-2.70866	3.29788	0.935501
N	-2.79065	-1.39087	-1.32565
N	-0.60247	-2.00835	-1.31031
N	4.77455	-2.37196	-2.83871
N	2.072944	-1.28368	2.589909
N	3.232642	0.177852	1.275019
N	0.325059	-5.95038	5.159348

O	-1.83603	-2.24666	-3.2426
O	5.570848	-2.83662	-2.03047
O	5.104934	-1.95146	-3.9439
O	4.22297	-1.79605	1.948167
O	-0.88519	-6.109	5.282105
O	1.15355	-6.75532	5.572539
O	0.438744	0.684212	1.801666
O	-1.16953	-0.65841	1.03994

2·HSO_4^- **W** conformation

Energy = -3518.695298

Sum of electronic and zero-point Energies = -3517.822249

Imaginary Frequencies = 0

Atom	X	Y	Z
H	6.605476	-0.15082	-0.51133
H	8.229963	-1.44408	-0.56068
H	-7.6226	-0.519	1.138989
H	-5.58326	0.234641	1.013409
H	-3.93592	-2.90866	0.292019
H	-2.84675	-5.13997	-0.05344
H	1.667016	-6.49448	-0.89274
H	-0.76508	-6.44682	-0.51182
H	3.836374	-5.26625	-1.10697
H	5.065107	-3.09288	-1.08497
H	7.984353	3.27488	-0.06791
H	6.527769	5.225478	-0.03073
H	3.100239	2.697874	-0.55233
H	1.925818	4.414716	0.32148
H	2.135109	4.598837	-1.43283
H	1.737136	5.99863	-0.43122
H	4.997461	6.366555	1.310988
H	3.640358	5.407285	1.923944
H	3.345608	6.983486	1.164075
H	4.142917	5.899405	-2.34897
H	5.287273	6.675897	-1.24187
H	3.625255	7.267638	-1.34564
H	9.520023	-3.25672	-0.62959
H	11.74126	-4.30392	-0.36847
H	13.42535	-0.49188	0.63629
H	11.20373	0.574226	0.373825
H	-6.44637	3.740061	0.749835

H	-4.83727	5.561807	0.627524
H	-1.65508	2.713001	0.207744
H	-0.48637	4.268169	1.345258
H	-1.46812	5.287474	2.410911
H	-0.23901	6.017017	1.359499
H	-0.61062	6.130928	-1.16147
H	-0.83295	4.377581	-1.19802
H	-2.08076	5.438653	-1.87416
H	-1.88181	7.566785	0.390004
H	-3.39468	7.01609	-0.33645
H	-3.16654	6.93031	1.422728
H	-9.18478	1.108536	-1.83287
H	-11.275	0.206196	-2.81333
H	-11.3769	-2.86624	0.174844
H	-9.27991	-1.98036	1.15563
H	-6.69267	-3.48721	0.812917
C	-2.07851	-1.83897	-0.0038
C	-2.87881	-3.00321	0.074958
C	-2.2708	-4.2208	-0.10153
C	-0.88162	-4.28305	-0.34006
C	-0.17142	-3.06212	-0.37372
C	1.271785	-3.09139	-0.58064
C	1.912999	-4.33778	-0.76553
C	1.148364	-5.55252	-0.74468
C	-0.19073	-5.52591	-0.53574
C	3.310333	-4.32861	-0.95723
C	3.991294	-3.13643	-0.94593
C	3.25511	-1.94733	-0.74133
C	3.915113	-0.67315	-0.68605
C	4.405808	0.431363	-0.59735
C	4.992022	1.726122	-0.46363
C	6.389162	1.862813	-0.33055
C	6.917978	3.147091	-0.17741
C	6.072794	4.247608	-0.15728
C	4.681797	4.14054	-0.29109
C	4.166006	2.859469	-0.44445
C	3.802276	5.395559	-0.25242
C	2.317039	5.071484	-0.46213
C	3.95976	6.077758	1.119892
C	4.245657	6.365441	-1.36396
C	8.506829	0.558354	-0.17886
C	10.21029	-1.2659	-0.14435

C	10.37425	-2.64715	-0.35242
C	11.61201	-3.24155	-0.20839
C	12.7009	-2.45068	0.147939
C	12.56267	-1.08398	0.358981
C	11.32164	-0.48616	0.214053
C	-2.66625	-0.53837	0.142205
C	-3.13026	0.573714	0.255131
C	-3.61983	1.90933	0.379762
C	-4.99407	2.181182	0.53292
C	-5.39546	3.512756	0.624196
C	-4.4676	4.545705	0.55239
C	-3.09856	4.301357	0.404829
C	-2.70336	2.967323	0.327766
C	-2.04641	5.413745	0.308956
C	-0.99901	5.231227	1.423626
C	-1.35235	5.331304	-1.06422
C	-2.66811	6.808824	0.455629
C	-7.13428	1.133343	-0.0084
C	-9.08735	-0.37809	-0.27448
C	-9.65869	0.240328	-1.40099
C	-10.8292	-0.26169	-1.94471
C	-11.4371	-1.3746	-1.37331
C	-10.8894	-2.00107	-0.25568
C	-9.72227	-1.5044	0.287131
N	-0.76723	-1.86598	-0.21593
N	1.93862	-1.92298	-0.57156
N	7.151947	0.688853	-0.36768
N	8.92471	-0.75718	-0.30691
N	14.0066	-3.06789	0.302339
N	-7.90347	0.030252	0.323372
N	-5.91368	1.122905	0.627606
N	-12.6614	-1.89258	-1.95028
O	9.260783	1.486654	0.07092
O	14.10385	-4.27477	0.111135
O	14.95291	-2.35536	0.616837
O	-7.49761	2.0163	-0.77498
O	-13.1778	-2.87813	-1.43331
O	-13.13	-1.32483	-2.93169
O	-7.49124	-1.70852	2.615988
O	-5.23437	-1.49375	1.708543
O	-5.5994	-2.78798	3.792968
O	-6.33939	-3.70714	1.686249

S	-6.14564	-2.31583	2.527475

2·HSO_4^- **U** conformation

Energy = -3518.743355

Sum of electronic and zero-point Energies = -3517.868734

Imaginary Frequencies = 0

Atom	X	Y	Z
H	-2.15004	-0.12313	-1.82391
H	-0.37197	-1.05689	-2.21018
H	0.308416	-0.32402	0.692309
H	2.149393	0.296165	0.44775
H	4.34836	5.367531	1.320681
H	3.023209	7.463227	1.557936
H	-1.62253	8.5024	0.896031
H	0.787238	8.624241	1.387456
H	-3.63416	7.12273	0.253313
H	-4.56814	4.890949	-0.34181
H	-4.61042	-2.84987	-1.88354
H	-6.93432	-2.60755	-1.22269
H	-6.20252	1.479568	-0.15656
H	-8.44335	1.729112	-0.42506
H	-7.9961	1.230455	1.220698
H	-9.64608	0.990362	0.636628
H	-8.98092	-1.75696	-1.77157
H	-8.98225	-0.03609	-2.19095
H	-10.2063	-0.68394	-1.08344
H	-7.86809	-1.25299	1.81278
H	-8.32235	-2.4816	0.622671
H	-9.55353	-1.39163	1.274983
H	1.857161	-1.43059	-2.28351
H	3.798405	-2.85155	-1.73495
H	1.167695	-5.891	-0.24453
H	-0.79303	-4.4815	-0.801
H	4.294887	-2.63728	0.944018
H	6.696786	-2.58452	0.5872
H	6.531054	1.673145	0.074635
H	8.169445	1.174202	-1.49605
H	8.172111	-0.48232	-2.12169
H	9.680542	0.25643	-1.54987
H	10.06545	0.636427	0.925923
H	8.575047	1.580116	1.030546

H	8.817379	0.19453	2.106913
H	10.09609	-1.63834	-0.00426
H	8.883245	-2.18378	1.160083
H	8.635987	-2.45062	-0.57801
H	0.353938	-3.66771	2.309154
H	-1.7776	-4.82662	2.858984
H	-4.00352	-1.40194	1.548752
H	-1.88899	-0.23285	1.019309
H	0.818678	3.27959	-1.04895
C	2.650513	4.227761	0.608526
C	3.292403	5.395075	1.081198
C	2.554387	6.546084	1.215803
C	1.173043	6.535	0.927691
C	0.617405	5.317644	0.485735
C	-0.8132	5.22793	0.242075
C	-1.60219	6.387711	0.392206
C	-0.99295	7.62424	0.794028
C	0.334905	7.692766	1.062998
C	-2.98778	6.255765	0.159973
C	-3.50755	5.02864	-0.16871
C	-2.62854	3.920927	-0.26429
C	-3.1706	2.61906	-0.54092
C	-3.71537	1.553178	-0.73525
C	-4.52996	0.387273	-0.89414
C	-4.04504	-0.8437	-1.37626
C	-4.95463	-1.90151	-1.5004
C	-6.27582	-1.75072	-1.11658
C	-6.77773	-0.54439	-0.60918
C	-5.88285	0.512518	-0.52617
C	-8.24363	-0.43807	-0.17718
C	-8.59257	0.962755	0.342477
C	-9.1541	-0.75051	-1.37961
C	-8.5098	-1.45467	0.949396
C	-1.98426	-2.16083	-1.61
C	0.394501	-2.86438	-1.5851
C	1.700954	-2.41824	-1.86039
C	2.791973	-3.20313	-1.54867
C	2.584963	-4.45038	-0.96405
C	1.302849	-4.91944	-0.70222
C	0.206092	-4.13376	-1.01259
C	3.368739	2.992357	0.485051
C	3.9663	1.937952	0.462118

C	4.680407	0.698675	0.465886
C	4.016217	-0.52766	0.708
C	4.782205	-1.69198	0.755413
C	6.157252	-1.64518	0.5514
C	6.834612	-0.45073	0.294413
C	6.064125	0.711144	0.260585
C	8.346882	-0.37223	0.051574
C	8.604101	0.178922	-1.36386
C	8.985199	0.567956	1.091807
C	9.02069	-1.74592	0.16618
C	1.829361	-1.49624	1.381855
C	-0.62632	-1.87906	1.622405
C	-0.59622	-3.17776	2.156564
C	-1.78431	-3.82121	2.457657
C	-2.99785	-3.17815	2.231989
C	-3.04921	-1.88405	1.719592
C	-1.86597	-1.23876	1.427866
N	1.35816	4.209576	0.295231
N	-1.32137	4.022893	-0.0734
N	-2.69411	-0.97822	-1.72212
N	-0.63938	-1.98085	-1.86801
N	3.727437	-5.26214	-0.60048
N	0.494079	-1.16512	1.240789
N	2.629355	-0.50779	0.851103
N	-4.23552	-3.87147	2.523603
O	-2.48526	-3.23824	-1.32352
O	4.851492	-4.79855	-0.77314
O	3.527695	-6.3779	-0.13123
O	2.240156	-2.51154	1.928232
O	-5.29485	-3.29355	2.300345
O	-4.1745	-5.00901	2.979915
O	2.021766	0.806561	-2.29311
O	-0.41564	0.795612	-2.5696
O	0.732045	2.878453	-1.96704
O	0.553849	1.091395	-0.32609
S	0.738203	1.299242	-1.78393

2·$H_2PO_4^-$ **W** conformation

Energy = -3462.612555

Sum of electronic and zero-point Energies = -3461.730125

Imaginary Frequencies = 0

Atom	X	Y	Z
H	6.628166	-0.14721	-0.40895
H	8.264807	-1.4268	-0.41372
H	-7.18438	-0.90994	0.210474
H	-5.51308	0.135494	0.243705
H	-3.98485	-2.88517	-0.36706
H	-2.87811	-5.12262	-0.65412
H	1.685666	-6.4913	-1.11563
H	-0.76922	-6.43484	-0.93871
H	3.870633	-5.27087	-1.1434
H	5.10229	-3.10417	-0.99859
H	7.967302	3.287057	0.078629
H	6.49566	5.226745	0.092542
H	3.09904	2.674709	-0.50638
H	1.898749	4.381297	0.364853
H	2.129484	4.568104	-1.38644
H	1.706921	5.963999	-0.38999
H	4.940247	6.36274	1.39307
H	3.584713	5.391625	1.990864
H	3.284687	6.96338	1.223964
H	4.139619	5.87945	-2.27602
H	5.26495	6.664297	-1.15535
H	3.600808	7.24633	-1.28208
H	9.572374	-3.22913	-0.43887
H	11.7995	-4.25184	-0.13671
H	13.43008	-0.41573	0.86453
H	11.20278	0.626003	0.560291
H	-6.50431	3.703207	0.356999
H	-4.89876	5.526556	0.382922
H	-1.69365	2.715806	-0.08793
H	-0.57642	4.227432	1.183316
H	-1.60239	5.196881	2.25318
H	-0.33736	5.975011	1.281755
H	-0.60864	6.198248	-1.23913
H	-0.82249	4.447903	-1.36471
H	-2.04594	5.536293	-2.04192
H	-1.95391	7.559765	0.309376
H	-3.439	7.029216	-0.48676
H	-3.26629	6.874783	1.273917
H	-9.93705	1.41896	-0.81799
H	-12.2523	0.588247	-1.12726
H	-11.0192	-3.35109	0.036984

H	-8.70512	-2.52801	0.363371
H	-7.14999	-2.83154	3.412855
H	-4.00034	-3.63965	2.343142
C	-2.09765	-1.83301	-0.43959
C	-2.9107	-2.98958	-0.47766
C	-2.29465	-4.2073	-0.62504
C	-0.88979	-4.27413	-0.7356
C	-0.17277	-3.05767	-0.67841
C	1.282207	-3.09209	-0.77215
C	1.930528	-4.33847	-0.93077
C	1.161276	-5.5489	-0.99279
C	-0.19044	-5.51735	-0.89613
C	3.338363	-4.33328	-1.01703
C	4.021077	-3.14467	-0.93755
C	3.27628	-1.95511	-0.77059
C	3.934343	-0.68357	-0.66007
C	4.420882	0.420012	-0.54185
C	4.995914	1.717	-0.38312
C	6.388734	1.863867	-0.22049
C	6.904251	3.151737	-0.05203
C	6.050695	4.245765	-0.04541
C	4.663516	4.128596	-0.20728
C	4.161025	2.844231	-0.37594
C	3.774429	5.377135	-0.18331
C	2.294798	5.041706	-0.41322
C	3.90792	6.063444	1.189471
C	4.226753	6.347778	-1.29059
C	8.513999	0.578424	-0.02749
C	10.23539	-1.22764	0.04018
C	10.41613	-2.60871	-0.15411
C	11.65735	-3.18967	0.013339
C	12.73268	-2.38522	0.380171
C	12.57769	-1.01857	0.578681
C	11.33327	-0.43422	0.409944
C	-2.69371	-0.53696	-0.28691
C	-3.15814	0.574003	-0.15991
C	-3.65798	1.902207	-0.0094
C	-5.0434	2.155637	0.111498
C	-5.45188	3.483104	0.256947
C	-4.52066	4.517065	0.267336
C	-3.14763	4.290745	0.144088
C	-2.7459	2.962966	0.01195

C	-2.10017	5.410794	0.137293
C	-1.09564	5.185082	1.283095
C	-1.35053	5.393472	-1.20874
C	-2.73635	6.795075	0.319308
C	-7.27683	1.110918	-0.12534
C	-9.16112	-0.50158	-0.21972
C	-10.1739	0.381867	-0.63515
C	-11.4667	-0.0835	-0.80565
C	-11.7593	-1.42228	-0.56569
C	-10.7716	-2.31408	-0.14904
C	-9.48326	-1.85307	0.022567
N	-0.77276	-1.86168	-0.53474
N	1.951061	-1.92744	-0.69453
N	7.162585	0.696747	-0.24704
N	8.94792	-0.73254	-0.14838
N	14.04204	-2.98806	0.55871
N	-7.83839	-0.14672	-0.03387
N	-5.9187	1.06568	0.110844
N	-13.1148	-1.89849	-0.74928
O	9.252896	1.513414	0.241694
O	14.15472	-4.19489	0.375897
O	14.97583	-2.26401	0.884179
O	-7.90252	2.13342	-0.38137
O	-13.3523	-3.08208	-0.52852
O	-13.9702	-1.09973	-1.11842
O	-5.78383	-1.83379	0.543742
O	-7.12293	-2.64359	2.468257
O	-4.90383	-3.72775	2.021616
O	-4.92862	-1.34656	2.967493
P	-5.61235	-2.25132	1.993056

2·$H_2PO_4^-$ **U** conformation

Energy = -3462.653086

Sum of electronic and zero-point Energies = -3461.768083

Imaginary Frequencies = 0

Atom	X	Y	Z
H	-2.36919	0.559287	-0.40176
H	-1.89845	2.483381	-1.32457
H	1.363462	-1.24026	-1.26745
H	3.126731	-0.40242	-1.20918
H	5.619619	1.548898	3.458621

H	4.638983	2.074955	5.690668
H	0.276462	1.763397	7.539611
H	2.687227	2.161299	7.165304
H	-1.88056	0.977029	6.730491
H	-3.26901	0.046239	4.875292
H	-4.9037	-0.59	-2.67861
H	-6.32093	-2.5466	-2.3326
H	-4.76336	-2.97157	1.644701
H	-6.66584	-4.07833	2.081365
H	-5.44643	-5.17062	1.383614
H	-7.15993	-5.60751	1.351457
H	-8.28346	-3.12772	-1.18323
H	-8.27383	-2.81923	0.56058
H	-8.79523	-4.39692	-0.06146
H	-5.39718	-5.57926	-1.12745
H	-6.54307	-4.75387	-2.20464
H	-7.12444	-5.98385	-1.0791
H	-1.05175	4.482723	-1.63517
H	-1.33631	6.91461	-2.07569
H	-5.58752	6.384273	-2.21991
H	-5.31196	3.958225	-1.7885
H	5.370193	-2.24904	-3.38938
H	7.773027	-1.83755	-3.50022
H	7.503503	0.694949	-0.04405
H	9.152169	1.841636	-1.1431
H	9.12097	1.653844	-2.90387
H	10.65075	1.503195	-2.01846
H	11.07581	-0.52118	-0.52908
H	9.575835	-0.20956	0.354538
H	9.849103	-1.79465	-0.38517
H	11.1183	-0.7104	-2.98373
H	9.94751	-2.03177	-2.9297
H	9.651207	-0.61871	-3.9651
H	1.826181	-4.82571	-2.17122
H	0.033333	-6.49934	-1.78496
H	-2.47926	-3.44839	-0.1209
H	-0.70021	-1.76481	-0.5024
H	-0.32366	0.38722	1.283936
H	1.586227	1.763791	1.408361
C	3.697097	1.026147	2.611397
C	4.558079	1.451672	3.648581
C	4.01398	1.734269	4.871547

C	2.630439	1.56121	5.080552
C	1.84185	1.126138	3.989165
C	0.417733	0.881744	4.209234
C	-0.10283	1.104144	5.508089
C	0.728024	1.591691	6.56824
C	2.04637	1.809065	6.363815
C	-1.45998	0.809753	5.744321
C	-2.22615	0.300044	4.732497
C	-1.62864	0.112479	3.467201
C	-2.43877	-0.42314	2.412764
C	-3.17738	-0.86638	1.563045
C	-4.01467	-1.3318	0.503346
C	-4.04624	-0.63311	-0.71529
C	-4.87773	-1.11017	-1.72924
C	-5.67692	-2.22179	-1.52124
C	-5.67918	-2.92492	-0.30673
C	-4.82246	-2.46724	0.687828
C	-6.63819	-4.10472	-0.1082
C	-6.45785	-4.77297	1.261033
C	-8.08347	-3.57726	-0.20603
C	-6.40656	-5.16563	-1.20044
C	-3.82446	1.702872	-1.33514
C	-3.16217	4.059607	-1.67685
C	-2.04029	4.91069	-1.76383
C	-2.19517	6.259032	-2.00911
C	-3.4795	6.777172	-2.17041
C	-4.60096	5.957727	-2.09033
C	-4.44889	4.603696	-1.84535
C	4.286133	0.686126	1.350711
C	4.933981	0.317946	0.394661
C	5.683904	-0.1959	-0.70744
C	5.05536	-1.02314	-1.66289
C	5.838112	-1.60514	-2.65585
C	7.206985	-1.36297	-2.70719
C	7.849208	-0.52454	-1.79022
C	7.058478	0.049649	-0.79482
C	9.354806	-0.23335	-1.82946
C	9.578665	1.283084	-1.9814
C	9.998716	-0.7184	-0.51662
C	10.04956	-0.94408	-2.99875
C	2.994629	-2.3658	-1.76851
C	0.687755	-3.18785	-1.35847

C	0.886618	-4.53025	-1.72905
C	-0.11312	-5.46193	-1.51185
C	-1.30936	-5.06288	-0.92441
C	-1.53555	-3.73473	-0.56799
C	-0.54394	-2.8015	-0.79035
N	2.379742	0.895751	2.768862
N	-0.35532	0.406333	3.20257
N	-3.25995	0.518515	-0.89899
N	-2.90401	2.725895	-1.40282
N	-3.64806	8.192668	-2.42517
N	1.641888	-2.19873	-1.51445
N	3.669861	-1.18431	-1.58637
N	-2.33478	-6.04865	-0.66142
O	-5.0092	1.809586	-1.62874
O	-2.64533	8.897857	-2.48541
O	-4.7856	8.630077	-2.56954
O	3.521708	-3.42144	-2.09831
O	-3.29157	-5.71716	0.033864
O	-2.20526	-7.17272	-1.13445
O	-0.21296	2.311106	-1.39879
O	1.621763	0.534077	-1.04109
O	-0.5293	0.482028	0.326419
O	1.149027	2.331961	0.733597
P	0.551362	1.423917	-0.4541

3·Cl^- **L-CH** conformation

Energy = -1832.351845

Sum of electronic and zero-point Energies = -1831.926134

Imaginary Frequencies = 0

Atom	X	Y	Z
H	-0.19302	0.352378	0.812991
H	1.837161	0.498457	0.933834
H	-2.18349	7.403947	-0.92644
H	-0.21649	6.249422	0.124594
H	-0.33685	3.767314	0.480662
H	-0.79137	-3.22815	0.5908
H	-3.0021	-4.22781	0.358275
H	-4.70185	-0.33051	-0.22573
H	-6.62502	-1.29815	0.482859
H	-7.49968	-2.52932	-0.43442
H	-6.38133	-1.44794	-1.2704

H	-4.64149	-4.79027	-1.16375
H	-5.16217	-3.47367	-2.22726
H	-6.36642	-4.49254	-1.41628
H	-5.78398	-3.1429	2.046471
H	-5.00825	-4.59186	1.386448
H	-6.72736	-4.30234	1.090251
H	3.912694	1.258975	1.150111
H	6.349637	1.017497	0.756729
H	5.647994	-2.67013	-1.31382
H	3.207279	-2.44051	-0.92191
H	-4.15674	6.039861	-1.57133
C	-3.28902	5.566978	-1.11781
C	-2.18397	6.333428	-0.75647
C	-1.09659	5.690465	-0.17558
C	-1.15247	4.316265	0.018215
C	-2.30773	3.636134	-0.38387
C	-2.40102	2.212921	-0.20821
C	-2.47182	1.012011	-0.06723
C	-2.59471	-0.40498	0.07239
C	-1.46559	-1.21132	0.30544
C	-1.64769	-2.59357	0.408733
C	-2.9092	-3.14944	0.270534
C	-4.05137	-2.36821	0.040703
C	-3.86425	-0.99446	-0.04825
C	-5.42435	-3.03442	-0.10403
C	-6.54096	-2.00988	-0.34458
C	-5.39228	-4.00615	-1.29903
C	-5.75112	-3.81511	1.183244
C	0.986158	-1.1678	0.082463
C	3.396503	-0.57617	0.139833
C	4.298205	0.399015	0.61155
C	5.654663	0.270535	0.395436
C	6.125666	-0.84149	-0.30044
C	5.255022	-1.81613	-0.777
C	3.893552	-1.68974	-0.56067
N	-3.36831	4.24657	-0.94447
N	-0.21135	-0.60573	0.466163
N	2.055598	-0.35564	0.404056
N	7.549237	-0.98412	-0.53158
O	1.083359	-2.25383	-0.47533
O	8.299883	-0.11623	-0.09737
O	7.944322	-1.96611	-1.1517

Cl	1.037191	2.14157	2.05771

3·Cl^- **L-N** conformation

Energy = -1832.349977

Sum of electronic and zero-point Energies = -1831.924081

Imaginary Frequencies = 0

Atom	X	Y	Z
H	0.204947	0.353082	0.717363
H	-1.81449	0.503885	0.887615
H	1.912634	7.396583	-0.87008
H	4.037511	6.477879	0.103111
H	4.238647	3.999925	0.394063
H	0.796468	-3.24029	0.485627
H	3.014261	-4.23055	0.289883
H	4.714637	-0.32436	-0.22796
H	6.414801	-1.43587	-1.25543
H	7.52178	-2.51635	-0.40295
H	6.627875	-1.29011	0.502254
H	5.001528	-4.58714	1.371198
H	5.763103	-3.13772	2.04665
H	6.725534	-4.29511	1.106973
H	5.221069	-3.46577	-2.23824
H	4.685598	-4.7853	-1.18592
H	6.413664	-4.48144	-1.40643
H	-3.87846	1.280108	1.1331
H	-6.32608	1.042393	0.805915
H	-5.69266	-2.69152	-1.20252
H	-3.24243	-2.46536	-0.87761
H	0.111616	5.809201	-1.503
C	1.041781	5.439415	-1.07869
C	2.050628	6.331598	-0.72479
C	3.225924	5.819359	-0.18714
C	3.343597	4.445559	-0.0239
C	2.271787	3.631409	-0.40914
C	2.365098	2.206444	-0.25338
C	2.471021	1.008154	-0.11387
C	2.601925	-0.40846	0.023265
C	1.46981	-1.21872	0.23013
C	1.653829	-2.60156	0.325502
C	2.920156	-3.15171	0.208766
C	4.065052	-2.36614	0.010103

C	3.875682	-0.99219	-0.0726
C	5.442488	-3.02807	-0.10998
C	6.560192	-1.99977	-0.32845
C	5.747088	-3.80925	1.182411
C	5.435927	-3.99843	-1.30647
C	-0.98977	-1.17978	0.043961
C	-3.39608	-0.57796	0.149071
C	-4.28164	0.411117	0.622691
C	-5.64357	0.28467	0.443257
C	-6.13695	-0.83954	-0.21663
C	-5.28269	-1.82815	-0.69412
C	-3.91564	-1.7036	-0.51492
N	1.13219	4.116612	-0.9333
N	0.217434	-0.6094	0.381701
N	-2.04844	-0.3576	0.375213
N	-7.56644	-0.98009	-0.40862
O	-1.10343	-2.27822	-0.48599
O	-8.30177	-0.09743	0.022087
O	-7.98183	-1.97523	-0.99357
Cl	-0.9925	2.14458	1.991214

3·OAc$^-$ **L-CH** conformation

Energy = -1600.558120

Sum of electronic and zero-point Energies = -1600.081126

Imaginary Frequencies = 0

Atom	X	Y	Z
H	-0.24441	0.286698	0.174622
H	1.686458	0.501781	0.219351
H	-1.9818	7.321481	-1.12232
H	0.008984	6.045034	-0.28206
H	-0.21454	3.559648	0.061614
H	-0.91001	-3.34099	0.163835
H	-3.15888	-4.27636	0.2021
H	-4.80802	-0.33739	-0.21757
H	-6.67752	-1.22366	0.66093
H	-7.67224	-2.46792	-0.10125
H	-6.61742	-1.45916	-1.09858
H	-4.98215	-4.86006	-0.99461
H	-5.59638	-3.59235	-2.06723
H	-6.7164	-4.52385	-1.05435
H	-5.69441	-2.98535	2.219094

H	-5.03637	-4.49522	1.567313
H	-6.77229	-4.17171	1.458459
H	3.741244	1.292616	0.447575
H	6.205836	1.010894	0.327575
H	5.672032	-3.00541	-1.07649
H	3.207078	-2.73634	-0.95061
H	0.73546	-0.09127	2.580929
H	2.37644	0.537499	2.688812
H	1.18951	0.965199	3.945156
H	-4.08321	6.078625	-1.58431
C	-3.20333	5.551834	-1.22268
C	-2.02681	6.250054	-0.96364
C	-0.92581	5.53857	-0.49947
C	-1.03612	4.166203	-0.31464
C	-2.26332	3.56002	-0.60904
C	-2.41661	2.140704	-0.43977
C	-2.53639	0.94286	-0.30411
C	-2.68569	-0.47059	-0.15722
C	-1.55501	-1.30554	-0.04588
C	-1.76317	-2.68346	0.080551
C	-3.04876	-3.20138	0.094052
C	-4.18944	-2.39255	-0.00818
C	-3.97522	-1.02537	-0.13301
C	-5.58746	-3.01994	0.039621
C	-6.69657	-1.97401	-0.13568
C	-5.72417	-4.06182	-1.0867
C	-5.78063	-3.71022	1.403451
C	0.915612	-1.33432	-0.28954
C	3.309653	-0.70516	-0.23903
C	4.172634	0.352851	0.117454
C	5.541637	0.202324	0.050814
C	6.067219	-1.01559	-0.37951
C	5.23683	-2.07238	-0.7417
C	3.862381	-1.92383	-0.67439
C	0.916066	2.00524	2.052278
C	1.325547	0.781311	2.878703
N	-3.33907	4.234996	-1.05598
N	-0.28922	-0.71395	-0.025
N	1.958679	-0.44787	-0.13382
N	7.503823	-1.18243	-0.4506
O	1.031835	-2.50999	-0.61711
O	8.21724	-0.23842	-0.12476

O	7.949387	-2.26003	-0.83305
O	0.564896	3.040641	2.631735
O	0.974785	1.862471	0.774847

3·OAc$^-$ **L-N** conformation

Energy = -1600.559346

Sum of electronic and zero-point Energies = -1600.083023

Imaginary Frequencies = 0

Atom	X	Y	Z
H	-0.17146	0.152022	0.85591
H	1.828876	0.578564	0.422046
H	-2.33204	7.17888	-1.18844
H	-4.55923	6.06865	-0.83693
H	-4.61214	3.594768	-0.48238
H	-0.69313	-3.3772	0.516359
H	-2.88618	-4.44013	0.386649
H	-4.69828	-0.60737	-0.27796
H	-6.58041	-1.58864	0.51134
H	-7.44725	-2.8837	-0.32076
H	-6.37809	-1.81768	-1.23845
H	-4.56407	-5.11789	-1.01182
H	-5.14664	-3.87121	-2.12658
H	-6.30181	-4.86833	-1.22308
H	-5.63449	-3.31724	2.140423
H	-4.85089	-4.78538	1.534163
H	-6.58559	-4.54673	1.284979
H	3.86817	1.341645	0.62042
H	6.326681	1.057542	0.388819
H	5.729773	-2.9755	-0.93769
H	3.274321	-2.69788	-0.71438
H	1.532938	4.227648	2.384929
H	-0.0522	4.332415	1.60484
H	0.065971	3.663952	3.242487
H	-0.28817	5.767672	-1.17398
C	-1.26586	5.316471	-1.02365
C	-2.41023	6.109394	-1.03186
C	-3.64061	5.491669	-0.83685
C	-3.6762	4.118018	-0.63979
C	-2.46949	3.406454	-0.64516
C	-2.47622	1.986455	-0.43924
C	-2.50648	0.79095	-0.24941

C	-2.58134	-0.62138	-0.04302
C	-1.42326	-1.38864	0.189725
C	-1.57175	-2.7721	0.3397
C	-2.82225	-3.36331	0.259424
C	-3.99084	-2.61805	0.042574
C	-3.83978	-1.24455	-0.10155
C	-5.3513	-3.32178	-0.02356
C	-6.49979	-2.33771	-0.28283
C	-5.33517	-4.35699	-1.16399
C	-5.61724	-4.03615	1.31527
C	1.008931	-1.27799	-0.08441
C	3.404466	-0.65941	-0.02985
C	4.286923	0.400764	0.278347
C	5.650624	0.246247	0.150773
C	6.159179	-0.97693	-0.28763
C	5.311347	-2.03672	-0.5972
C	3.941695	-1.88509	-0.47146
C	0.732259	2.346834	1.649444
C	0.567999	3.728245	2.275238
N	-1.27559	3.995296	-0.83832
N	-0.18816	-0.73678	0.308674
N	2.059104	-0.40653	0.145827
N	7.588808	-1.14561	-0.42138
O	1.132754	-2.39033	-0.59315
O	8.318355	-0.19924	-0.13794
O	8.017868	-2.2278	-0.81228
O	-0.08945	1.455092	1.983227
O	1.664531	2.202061	0.807787

3·HSO_4^- **L-CH** conformation

Energy = -2071.697332

Sum of electronic and zero-point Energies = -2071.242099

Imaginary Frequencies = 0

Atom	X	Y	Z
H	-0.21456	0.090813	-0.3017
H	1.749697	0.396272	-0.20379
H	-2.99004	7.004194	-1.34034
H	-0.72234	5.9398	-1.51023
H	-0.52991	3.470151	-1.09377
H	-0.69407	-3.58225	-0.11967
H	-2.88884	-4.60564	0.125264

H	-4.7251	-0.73702	-0.10186
H	-6.4697	-1.70863	0.944149
H	-7.48165	-2.9792	0.251884
H	-6.56348	-1.91378	-0.81763
H	-4.79552	-5.2492	-0.92739
H	-5.53889	-3.98478	-1.91977
H	-6.53896	-4.97166	-0.83642
H	-5.27993	-3.46424	2.371683
H	-4.63704	-4.9375	1.626924
H	-6.38473	-4.66956	1.682753
H	3.74332	1.229895	0.322469
H	6.217878	1.025041	0.341776
H	5.887418	-3.04364	-0.97025
H	3.413908	-2.841	-1.01687
H	-1.29322	1.601025	1.477858
H	-4.93859	5.569934	-0.78032
C	-3.94597	5.134995	-0.86645
C	-2.85378	5.941177	-1.17916
C	-1.6003	5.348346	-1.27336
C	-1.48471	3.981364	-1.05618
C	-2.6437	3.260529	-0.75223
C	-2.57732	1.839459	-0.53345
C	-2.55436	0.6348	-0.38997
C	-2.60325	-0.78585	-0.24066
C	-1.43209	-1.57234	-0.24687
C	-1.57563	-2.95903	-0.1146
C	-2.83313	-3.5262	0.019688
C	-4.01086	-2.76629	0.030543
C	-3.86224	-1.3922	-0.10067
C	-5.37288	-3.45005	0.190942
C	-6.53265	-2.44676	0.138218
C	-5.56848	-4.47561	-0.94193
C	-5.41709	-4.17427	1.550057
C	1.046575	-1.51238	-0.45046
C	3.417507	-0.78562	-0.36954
C	4.220866	0.304891	0.016379
C	5.595815	0.191936	0.040963
C	6.180138	-1.02135	-0.31793
C	5.406161	-2.11339	-0.69654
C	4.026242	-2.00058	-0.72631
N	-3.8629	3.821023	-0.65417
N	-0.19934	-0.92511	-0.35942

N	2.049216	-0.56619	-0.38658
N	7.624467	-1.14852	-0.29092
O	1.241186	-2.71487	-0.57056
O	8.28874	-0.17056	0.036182
O	8.121159	-2.2276	-0.59633
O	0.521244	3.666188	1.74221
O	1.857528	1.644831	2.26269
O	-0.54839	1.441696	2.082705
O	0.783531	1.895646	0.05693
S	0.757812	2.24227	1.508699

3·HSO_4^- **L-N** conformation

Energy = -2071.706042

Sum of electronic and zero-point Energies = -2071.250691

Imaginary Frequencies = 0

Atom	X	Y	Z
H	-0.22813	0.069784	-0.04796
H	1.732471	0.347967	-0.11496
H	-2.7494	7.004317	-1.44799
H	-4.31464	5.479795	-2.68631
H	-4.19184	3.025044	-2.24174
H	-0.76563	-3.58655	0.129179
H	-2.9797	-4.58416	0.299001
H	-4.76463	-0.70936	-0.1418
H	-6.5622	-1.63049	0.860752
H	-7.55632	-2.91095	0.160803
H	-6.57724	-1.88804	-0.8967
H	-4.84436	-5.24313	-0.82257
H	-5.53345	-4.00534	-1.8849
H	-6.58769	-4.95	-0.81472
H	-5.45934	-3.34582	2.394328
H	-4.79823	-4.84901	1.729953
H	-6.54373	-4.56441	1.696698
H	3.762915	1.134919	0.378971
H	6.232254	0.897522	0.275949
H	5.786518	-3.13028	-1.126
H	3.316963	-2.89734	-1.04862
H	-0.59908	3.662491	0.993246
H	-1.14712	5.993762	0.172171
C	-1.8414	5.372377	-0.38552
C	-2.73561	5.933042	-1.28859

C	-3.60074	5.085445	-1.97167
C	-3.53859	3.720283	-1.72871
C	-2.60807	3.239824	-0.80129
C	-2.53724	1.834001	-0.52943
C	-2.56266	0.63417	-0.36641
C	-2.63909	-0.78036	-0.17615
C	-1.47751	-1.57593	-0.10007
C	-1.64033	-2.95605	0.071171
C	-2.90806	-3.50929	0.160963
C	-4.07712	-2.73916	0.091199
C	-3.90898	-1.37099	-0.07869
C	-5.45246	-3.40466	0.21248
C	-6.59707	-2.39179	0.075068
C	-5.60934	-4.46465	-0.89427
C	-5.56617	-4.08209	1.591465
C	0.991702	-1.54804	-0.35084
C	3.377781	-0.85987	-0.35049
C	4.212559	0.21117	0.026157
C	5.585432	0.08073	-0.01737
C	6.137004	-1.12931	-0.43545
C	5.331728	-2.20223	-0.80409
C	3.953655	-2.07283	-0.76488
N	-1.77412	4.061528	-0.13904
N	-0.23438	-0.94303	-0.17286
N	2.014568	-0.62256	-0.29779
N	7.578905	-1.27288	-0.48192
O	1.156847	-2.74823	-0.53241
O	8.270269	-0.31211	-0.15945
O	8.047693	-2.34781	-0.84201
O	0.81722	1.827688	0.1717
O	2.247203	2.487857	2.071684
O	0.129491	1.281297	2.468507
O	0.13927	3.63317	1.680054
S	0.879769	2.212505	1.615774

3·$H_2PO_4^-$ **L-CH** conformation

Energy = -2015.613461

Sum of electronic and zero-point Energies = -2015.147973

Imaginary Frequencies = 0

Atom	X	Y	Z
H	-0.20849	0.139455	-0.16562

H	1.722653	0.367879	-0.01751
H	-2.27891	7.090934	-1.62506
H	-0.14403	5.884948	-1.08426
H	-0.25361	3.412278	-0.61644
H	-0.80735	-3.50943	-0.0457
H	-3.03479	-4.47354	0.142055
H	-4.76533	-0.5675	-0.24113
H	-6.57001	-1.46879	0.757492
H	-7.58681	-2.73392	0.06244
H	-6.60214	-1.72151	-1.0003
H	-4.91643	-5.10078	-0.94916
H	-5.59777	-3.85086	-2.00214
H	-6.65518	-4.78369	-0.92469
H	-5.47966	-3.20231	2.277713
H	-4.83974	-4.71096	1.605044
H	-6.58247	-4.40775	1.585825
H	3.760044	1.216252	0.229662
H	6.226431	0.965239	0.178127
H	5.781805	-3.11976	-1.04734
H	3.313155	-2.88145	-0.99387
H	0.865633	0.598082	3.543012
H	-1.4988	1.949533	1.47537
H	-4.39615	5.793848	-1.68361
C	-3.45616	5.297305	-1.456
C	-2.26982	6.026001	-1.42331
C	-1.08963	5.354669	-1.12377
C	-1.13747	3.989995	-0.87047
C	-2.38076	3.351287	-0.93218
C	-2.46897	1.937405	-0.68026
C	-2.53485	0.741173	-0.49024
C	-2.64181	-0.67137	-0.30236
C	-1.49078	-1.48548	-0.24531
C	-1.67293	-2.8647	-0.08679
C	-2.94799	-3.39872	0.012954
C	-4.10615	-2.60993	-0.03536
C	-3.91954	-1.24298	-0.19369
C	-5.48968	-3.25648	0.095792
C	-6.62131	-2.22761	-0.02975
C	-5.67104	-4.31157	-1.01198
C	-5.60061	-3.93566	1.474146
C	0.983805	-1.48966	-0.45876
C	3.369718	-0.81755	-0.37636

C	4.20827	0.267961	-0.049
C	5.580541	0.13493	-0.07685
C	6.133145	-1.09338	-0.43702
C	5.326775	-2.17777	-0.769
C	3.948945	-2.04625	-0.74144
N	-3.53106	3.986503	-1.21855
N	-0.2403	-0.87078	-0.31652
N	2.01055	-0.57798	-0.32001
N	7.57389	-1.24178	-0.4651
O	1.137973	-2.68359	-0.68827
O	8.265157	-0.27289	-0.1665
O	8.043595	-2.32901	-0.78559
O	1.444975	3.011206	2.647423
O	0.770366	0.524925	2.587277
O	-0.9495	2.380094	2.146161
O	0.816057	1.755213	0.425395
P	0.621153	2.008312	1.91307

3·$H_2PO_4^-$ **L-N** conformation

Energy = -2015.620428

Sum of electronic and zero-point Energies = -2015.154473

Imaginary Frequencies = 0

Atom	X	Y	Z
H	-0.11137	0.063289	-0.28764
H	1.789961	0.435893	-0.3067
H	-3.81045	6.782245	-1.20782
H	-5.46598	5.015269	-1.87934
H	-4.89216	2.621503	-1.459
H	-0.49262	-3.63158	-0.12454
H	-2.64378	-4.73737	0.135681
H	-4.61543	-0.9324	0.033095
H	-6.30183	-1.98578	1.095182
H	-7.28787	-3.27219	0.393995
H	-6.42994	-2.15127	-0.66862
H	-4.55528	-5.42023	-0.90333
H	-5.35447	-4.15296	-1.84805
H	-6.30451	-5.19836	-0.77517
H	-5.02391	-3.74413	2.450865
H	-4.35516	-5.1756	1.649276
H	-6.10819	-4.96156	1.751055
H	3.758168	1.302349	0.374488

H	6.2436	1.192245	0.387577
H	6.069599	-2.86528	-0.9895
H	3.590896	-2.75149	-1.04744
H	-1.06569	1.422597	1.626112
H	-0.5609	3.910914	0.611436
H	-1.67764	6.062245	-0.14493
C	-2.41788	5.330081	-0.45364
C	-3.60946	5.730386	-1.04531
C	-4.52278	4.749388	-1.41514
C	-4.21027	3.417029	-1.1841
C	-2.98422	3.104327	-0.58553
C	-2.66122	1.725002	-0.34965
C	-2.52732	0.523111	-0.25095
C	-2.49502	-0.90216	-0.13986
C	-1.29584	-1.64494	-0.19014
C	-1.39484	-3.04032	-0.08854
C	-2.62824	-3.65417	0.05602
C	-3.83166	-2.93719	0.106013
C	-3.73053	-1.55701	0.004272
C	-5.16639	-3.67057	0.273764
C	-6.35961	-2.70594	0.272719
C	-5.35129	-4.67043	-0.88355
C	-5.15861	-4.43411	1.611916
C	1.175904	-1.51615	-0.4091
C	3.515473	-0.70582	-0.37299
C	4.275645	0.407492	0.038202
C	5.65388	0.343117	0.066789
C	6.285177	-0.84213	-0.30839
C	5.553306	-1.95747	-0.70438
C	4.170651	-1.89371	-0.74062
N	-2.10295	4.052813	-0.22326
N	-0.08801	-0.96193	-0.32395
N	2.142419	-0.53338	-0.40628
N	7.732247	-0.91649	-0.27814
O	1.412254	-2.71732	-0.47143
O	8.36071	0.083564	0.054381
O	8.269857	-1.97543	-0.58673
O	0.738105	1.773552	-0.20056
O	2.145522	2.35429	1.918835
O	-0.25881	1.584266	2.134052
O	0.277328	3.884821	1.140979
P	0.836669	2.373047	1.199433

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