Electronic Supporting Information

Naphthalene strapped fluorescent Calix[4]pyrrole isomers: Halide ion selectivity based on strap topography

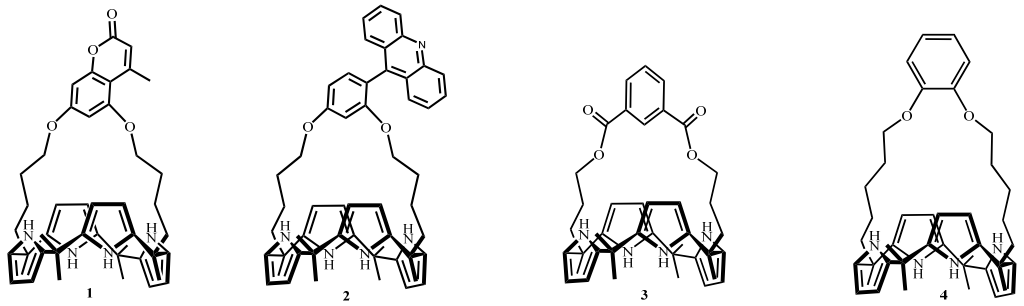
Ritwik Samanta, Sanjeev P. Mahanta, Susanta Ghanta and Pradeepta K. Panda*

School of Chemistry, University of Hyderabad, Hyderabad, Andhra Pradesh, India, 500046.

E-mail: pkpsc@uohyd.ernet.in,pradeepta.panda@gmail.com.

Instrumentation and reagents:

NMR spectra were recorded on a Bruker Avance-400 MHz and 500 MHz FT NMR spectrometer using tetramethylsilane (TMS, $\delta = 0$) as an internal standard at room temperature. Mass spectral determinations were carried out by Shimadzu-LCMS-2010 mass spectrometer and elemental analysis was obtained through Thermo Finnigan Flash EA 1112 analyzer. Melting points were determined by a MR-VIS+ visual melting point range apparatus from Labindia Instruments Pvt. Ltd. IR spectra were recorded on a JASCO-FT-IR model 5300 and NICOLET 5700 FT-IR spectrometer. Microcalorimetric titrations were performed using an isothermal titration calorimeter (ITC) purchased from Microcal Inc., MA. The Origin software provided by Microcal Inc. was used to calculate the binding constant (K_a) and the enthalpy change (ΔH). Fluorescence measurements were done by using a HORIBA Jobin Yvon Fluromax-4 instrument. The solvent acetonitrile was purchased from Sigma-Aldrich® and used as such. All tetrabutylammonium (TBA) salts for NMR and ITC titration were purchased from Sigma-Aldrich® and were directly used in the titration experiment. All quantum mechanical DFT calculations were performed with the Gaussian 03 program package.[S1] The restricted Becke three-parameter hybrid (B3)[S2] functional was used along with Lee-Yang-Parr (LYP)[S3] correction. The 6-31+G (d,p) basis set is employed in all calculations reported below.

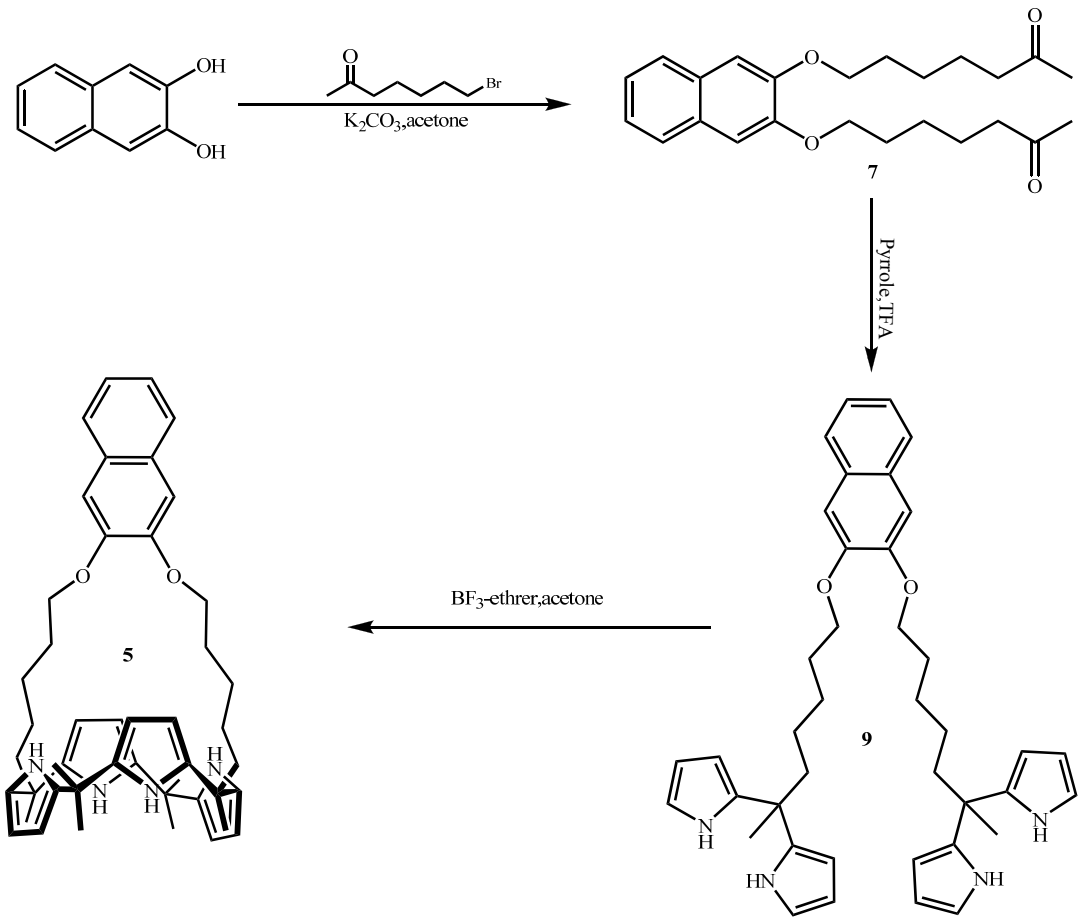


Synthesis of compound 7: A mixture of 2,3-dihydroxynaphthalene (480 mg, 3 mmol) and K_2CO_3 (4.14g, 30 mmol) in acetone (100 mL) was stirred well for about 1 h, and then 7-bromo-2-heptanone[S4] (2.89g, 15 mmol) was added. The mixture was refluxed for 3 days and then filtered and solvent was removed. The crude product was purified by column chromatography over silica gel with increasing ratio of ethyl acetate in hexane. The excess bromoketone is removed first (15 % ethyl acetate in hexane) and the desired

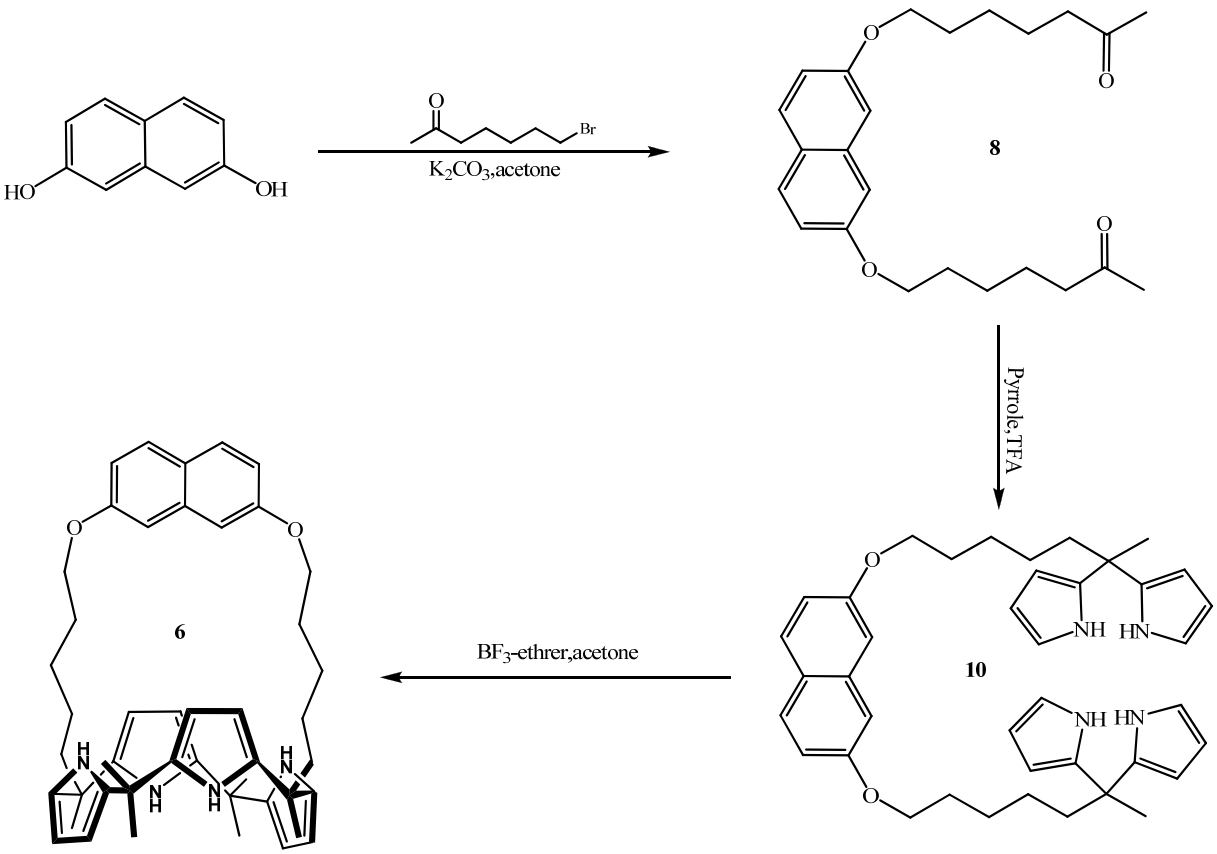
product was collected as the next major band and vacuum dried to give compound **7** as a white solid (900 mg; 78%). Melting point: 76.4°C IR(neat): ν (cm^{-1}) 2939.78-2860.69, 1714.87; ^{1}H NMR ($CDCl_3$): δ in ppm 7.65(m, 2H), 7.31(m, 2H), 7.10(s, 2H), 4.10(t, 4H, J = 6.4 Hz), 2.49(t, 4H, J = 7.6 Hz), 2.15(s, 6H), 1.91(m, 4H), 1.69(m,4H); ^{13}C NMR ($CDCl_3$): δ in ppm 209.11, 149.35, 129.35, 126.35, 108.00, 68.60, 43.75, 30.06, 29.04, 25.82, 23.67. LCMS m/z, M+H: 385.5 (calculated for $C_{24}H_{33}O_4$= 385.24). Anal.Calcd for $C_{24}H_{32}O_4$: C, 74.97; H, 8.39. Found: C, 74.84; H, 8.41.

Synthesis of compound 9: To a mixture of **7** (746 mg; 1.94 mmol) and pyrrole (5.4mL; 78 mmol), trifluoroacetic acid (150 µL; 1.94 mmol) was added at about 60°C and mixture was stirred for about 4 h at this temperature. Then reaction was quenched with triethylamine (1mL). Excess reagents were removed under reduced pressure to get the crude product, which was purified by column chromatography over silica gel (10 % ethyl acetate in hexane) to obtain the pure product as a dense mass**9**(750mg, 63 %). IR(neat): ν (cm^{-1}) 3391.16, 2932.06-2858.76, 1715; ^{1}H NMR ($CDCl_3$): δ in ppm 7.79(br s, 4H), 7.65(m, 2H), 7.3(m, 2H), 7.09(s, 2H), 6.59(s, 4H), 6.09(d, 8H, J = 18 Hz), 4.05(t, 4H, J=6.2 Hz), 1.99(m, 4H), 1.85(m, 4H), 1.58(s, 6H), 1.50(m, 4H), 1.28(m, 4H); ^{13}C NMR ($CDCl_3$): δ in ppm 149.43, 138.27, 129.37, 126.36, 124.14, 117.08, 107.83, 104.63, 68.85, 51.03, 41.29, 39.22, 29.03, 26.52, 24.31. LCMS m/z, M+H: 617.7(calculated for $C_{40}H_{48}N_4O_2$= 617.38). Anal.Calcd.for $C_{40}H_{48}N_4O_2$ C, 77.89; H, 7.84; N, 9.08.Found C, 77.95; H, 7.76; N, 8.96.

Scheme 1:



Scheme 2:



Synthesis of compound 5: To a solution of **9** (814 mg; 1.32 mmol) and acetone (150 mL), $BF_3.OEt_2$ (1 μL; 0.38 mmol) was added. The solution was stirred at room temperature for 15 min, after which product formation was confirmed by TLC. The reaction was quenched by triethylamine (1mL) and solvent was removed. The crude mass was subjected to column chromatography over silica gel (10 % ethyl acetate in hexane) to obtain the product as a colored species, which upon subsequent washing with methanol yielded the pure macrocycle **5** as an off white powder (106mg, 11%). Melting point: 178°C (decomp.) ^{1}H NMR ($CDCl_3$): δ in ppm 7.66(br s, 4H), 7.31(m, 2H), 7.10(s, 2H), 5.94(s, 8H), 4.09(t, 4H, J = 6 Hz), 1.92(m, 8H), 1.67(m, 8H), 1.52(m, 12H), 1.269m, 4H); ^{13}C NMR ($CDCl_3$): δ in ppm 149.46, 137.86, 137.21, 129.43, 126.40, 124.18, 108.16, 104.30, 103.69, 68.65, 41.35, 39.53, 35.62, 30.21, 29.21, 28.26, 26.66, 25.17.LCMS m/z, M+H: 697.75 (calculated for $C_{46}H_{56}N_4O_2$= 697.44). Anal.Calcd.for $C_{46}H_{56}N_4O_2.2CH_3OHC$, 75.75; H, 8.48; N, 7.36.Found C, 75.68; H, 8.55; N, 7.31.

Synthesis of compound 8: A mixture of 2,7-dihydroxynaphthalene (480 mg, 3 mmol) and K_2CO_3 (4.14g, 30 mmol) in acetone (100 mL) was stirred well for about 1 h, and then 7-bromo-2-heptanone (2.89g, 15 mmol) was added. The mixture was refluxed for 3 days and then filtered and solvent was removed. The crude product was purified by column chromatography over silica gel with increasing ratio of ethyl acetate in hexane. The excess bromoketone is removed first (15 % ethyl acetate in hexane) and the desired product was collected as the next major band and vacuum dried to give compound **8**as a white solid (970 mg; 84 %). Meltingpoint:61.8°C IR(neat): ν (cm^{-1}) 2939.78-2860.69, 1714.87; ^{1}H NMR ($CDCl_3$): δ in ppm 7.63(d, 2H, J = 9.2 Hz), 7.01(s, 2H), 6.98(d, 2H,), 4.06(t, 4H, J = 6.4 Hz), 2.49(t, 4H, J = 7.2 Hz), 2.15(s, 6H), 1.85(m, 4H), 1.67(m, 4H), 1.51(m, 4H) ; ^{13}C NMR ($CDCl_3$):209.12, 157.62, 136.00, 129.13, 124.23, 116.29, 106.05, 67.06, 43.66, 30.02, 29.14, 25.80, 23.58. LCMS m/z, M+H: 385.5 (calculated for $C_{24}H_{33}O_4$= 385.24). Anal.Calcd for $C_{24}H_{32}O_4$: C, 74.97; H, 8.39. Found: C, 74.84; H, 8.40.

Synthesis of compound 10: To a mixture of **8** (746 mg; 1.94 mmol) and pyrrole (5.4mL; 78 mmol), trifluoroacetic acid (150 µL; 1.94 mmol) was added at about 60°C and mixture was stirred for about 4 h at this temperature. Then reaction was quenched with triethylamine (1mL). Excess reagents were removed under reduced pressure to get the crude product, which was purified by column chromatography over silica gel (10 % ethyl acetate in hexane) to obtain the pure product **10**(665mg, 55 %). Melting point: starts decomposing slowly above 60°C.IR(neat): ν (cm^{-1}) 3391.16, 2932.06-2858.76, 1715; ^{1}H NMR ($CDCl_3$): δ in ppm 7.71(br s, 4H), 7.63(d, 2H), 6.98(m 4H), 6.60(s, 4H), 6.13(m, 8H), 4.01(t, 4H), 2.02(m, 4H), 1.81(m, 4H), 1.59(s, 6H), 1.48(m, 4H), 1.28(m, 4H); ^{13}C NMR ($CDCl_3$): δ in ppm 157.60, 138.15, 136.00, 12.07, 124.23, 117.01, 116.26, 107.68, 106.04, 67.88, 41.17, 39.04, 29.20, 26.64, 26.31, 24.28.LCMS m/z, M+H: 617.7(calculated for $C_{40}H_{48}N_4O_2$= 617.38). Anal.Calcd.for $C_{40}H_{48}N_4O_2$ C, 77.89; H, 7.84; N, 9.08.Found C, 77.75; H, 7.76; N, 9.15.

Synthesis of compound 6: To a solution of **10** (1.16 g; 2.64 mmol) and acetone (300 mL), $BF_3.OEt_2$ (5µL; 0.04 mmol) was added. The solution was stirred at room temperature for 10 min, after which product formation was confirmed by TLC. The reaction was quenched by triethylamine (1mL) and solvent was removed. The crude mass was subjected to column chromatography over silica gel (10 % ethyl acetate in hexane) to obtain the product as a colored species, which upon subsequent washing with methanol yielded the pure macrocycle**6**as an off white powder (78mg, 6%). Meltingpoint: 172°C(decomp.) ^{1}H NMR ($CDCl_3$): δ in ppm 7.71(d, 2H, J = 9.2 Hz), 7.17(s, 2H), 7.11(s, 4H), 7.04(dd, 2H), 5.78(d, 8H, J = 27.2 Hz), 4.20(t, 4H, J = 6.8 Hz), 1.86(m, 8H),1.47(s,6H), 1.42(s, 6H), 1.37(s, 6H), 1.25(m, 4H); ^{13}C NMR ($CDCl_3$): δ in ppm 157.64, 138.42, 136.93, 136.22, 129.44, 124.66, 116.76, 107.11, 104.01, 102.94, 67.47, 41.76, 39.30, 35.47, 31.00, 29.85, 28.09, 25.09, 23.98.LCMS m/z, M+H: 697.75 (calculated for $C_{46}H_{56}N_4O_2$= 697.44). Anal.Calcd.for $C_{46}H_{56}N_4O_2$ C, 79.27; H, 8.10; N, 8.04.Found C, 79.21; H, 8.31; N, 8.09.

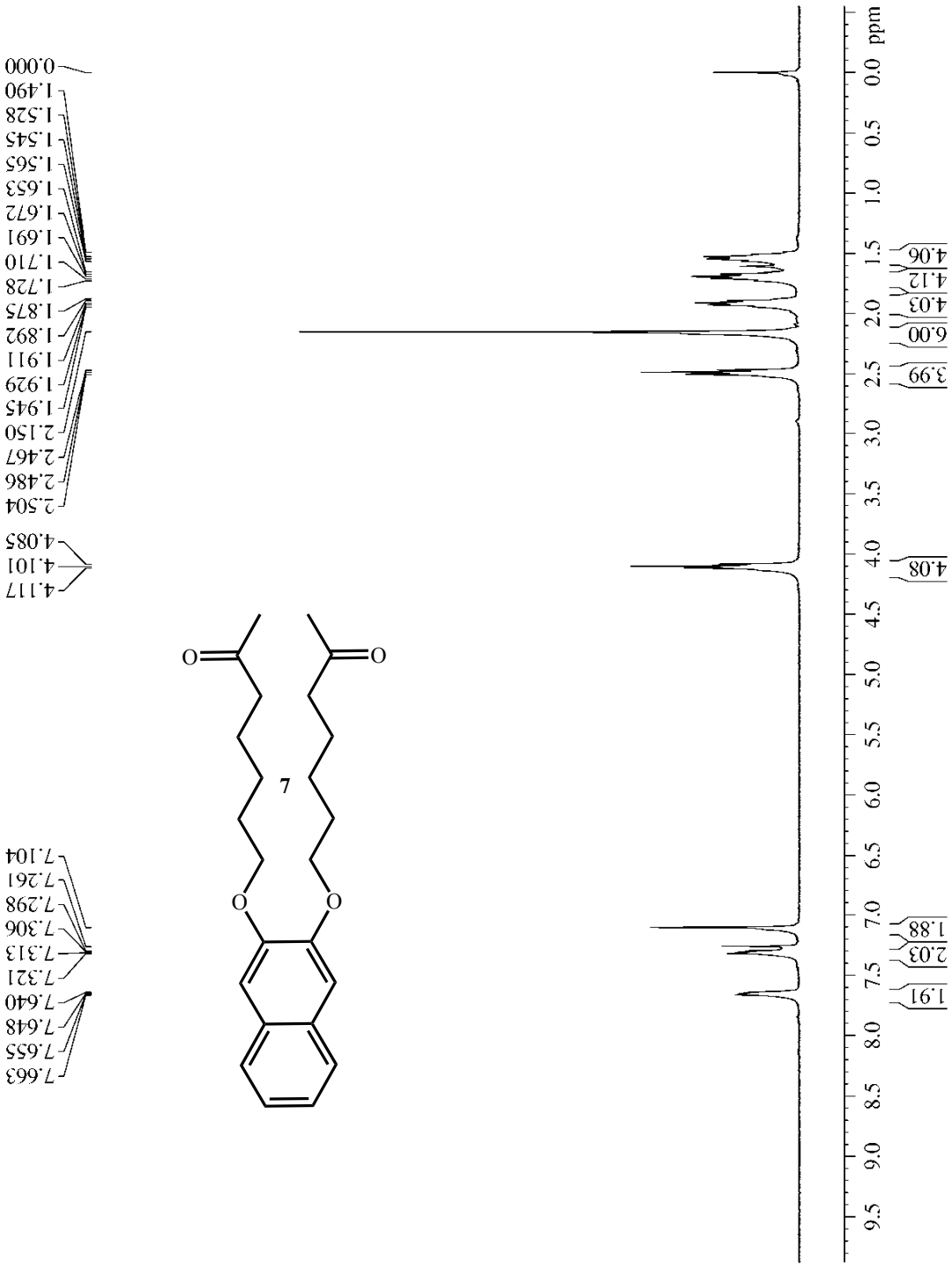


Fig S1:[1]H NMR of Compound **7** in $CDCl_3$.

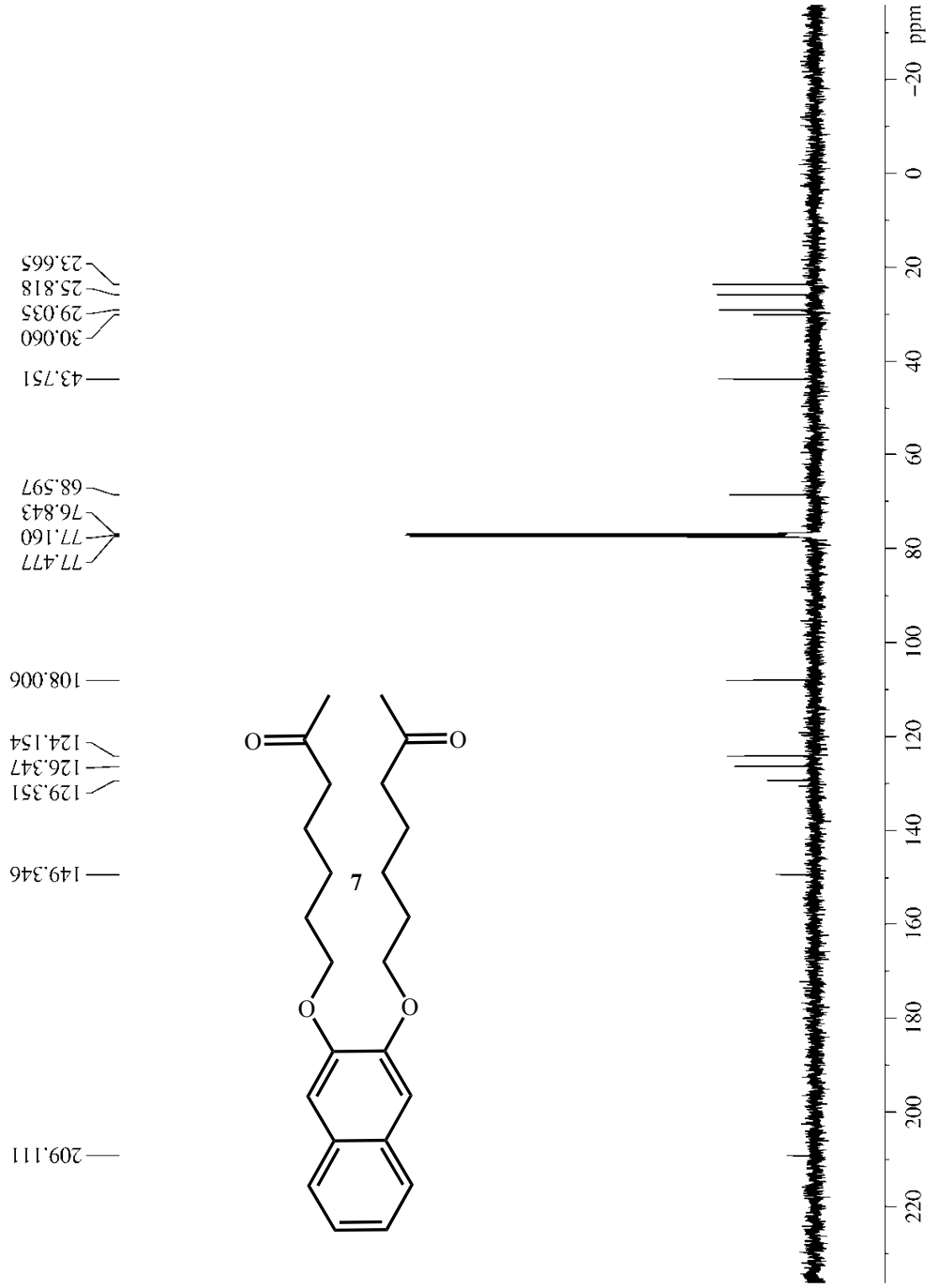


Fig S2:[13]C NMR of Compound **7** in $CDCl_3$.

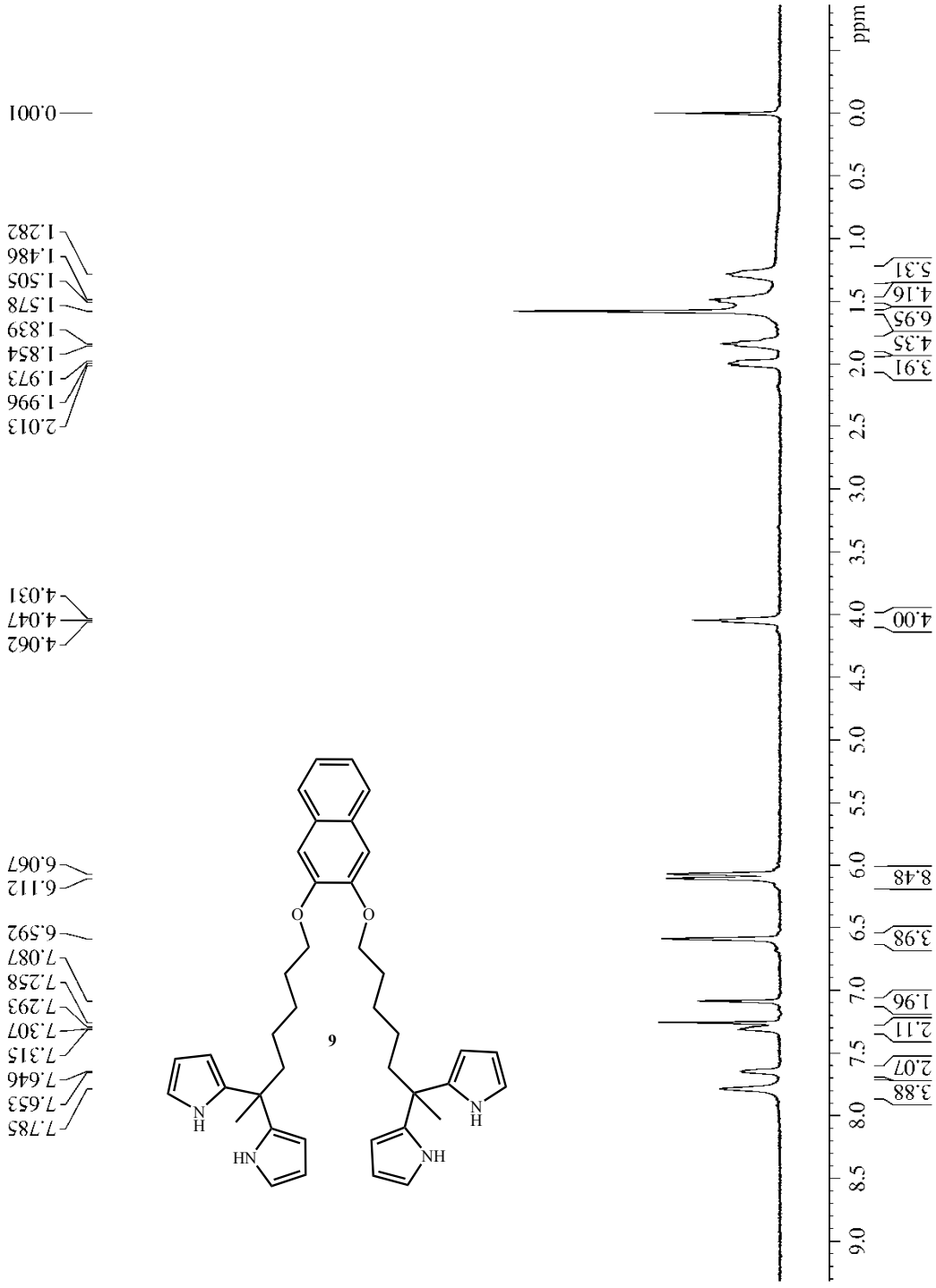


Fig S3:[1]H NMR of Compound **9** in $CDCl_3$.

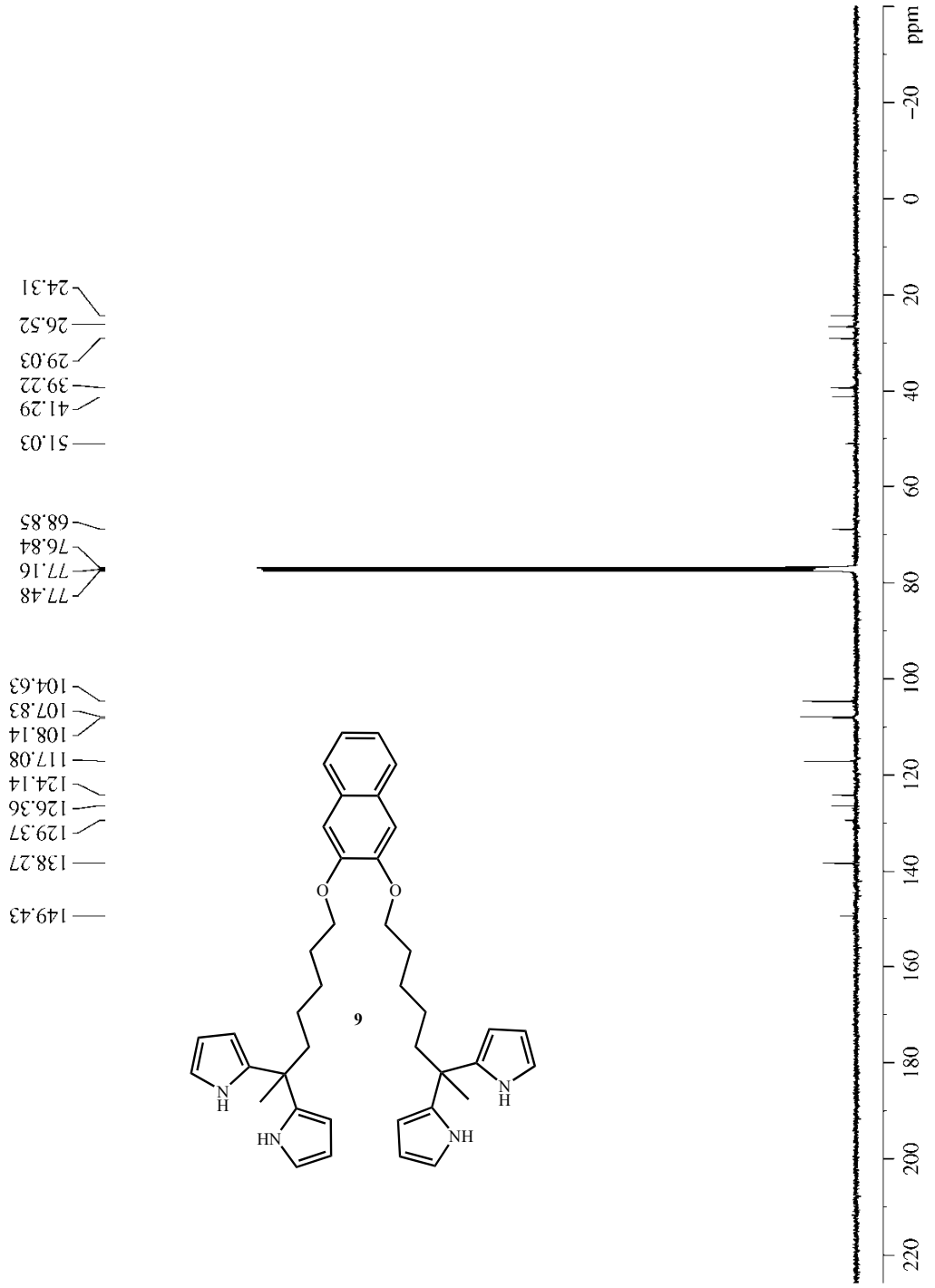


Fig S4:[13]CNMR of Compound **9** in $CDCl_3$.

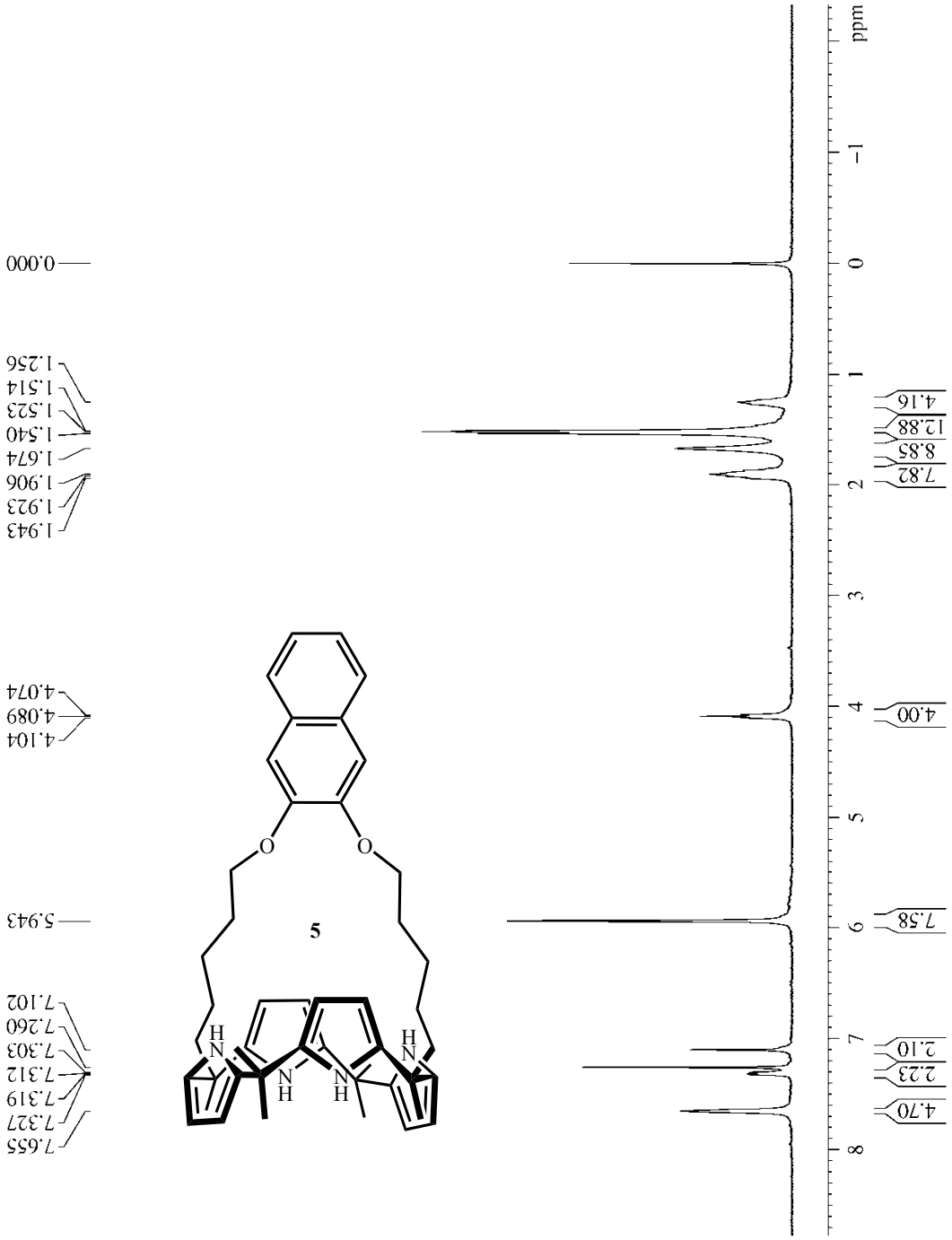


Fig S5:[1]H NMR of Compound **5** in $CDCl_3$.

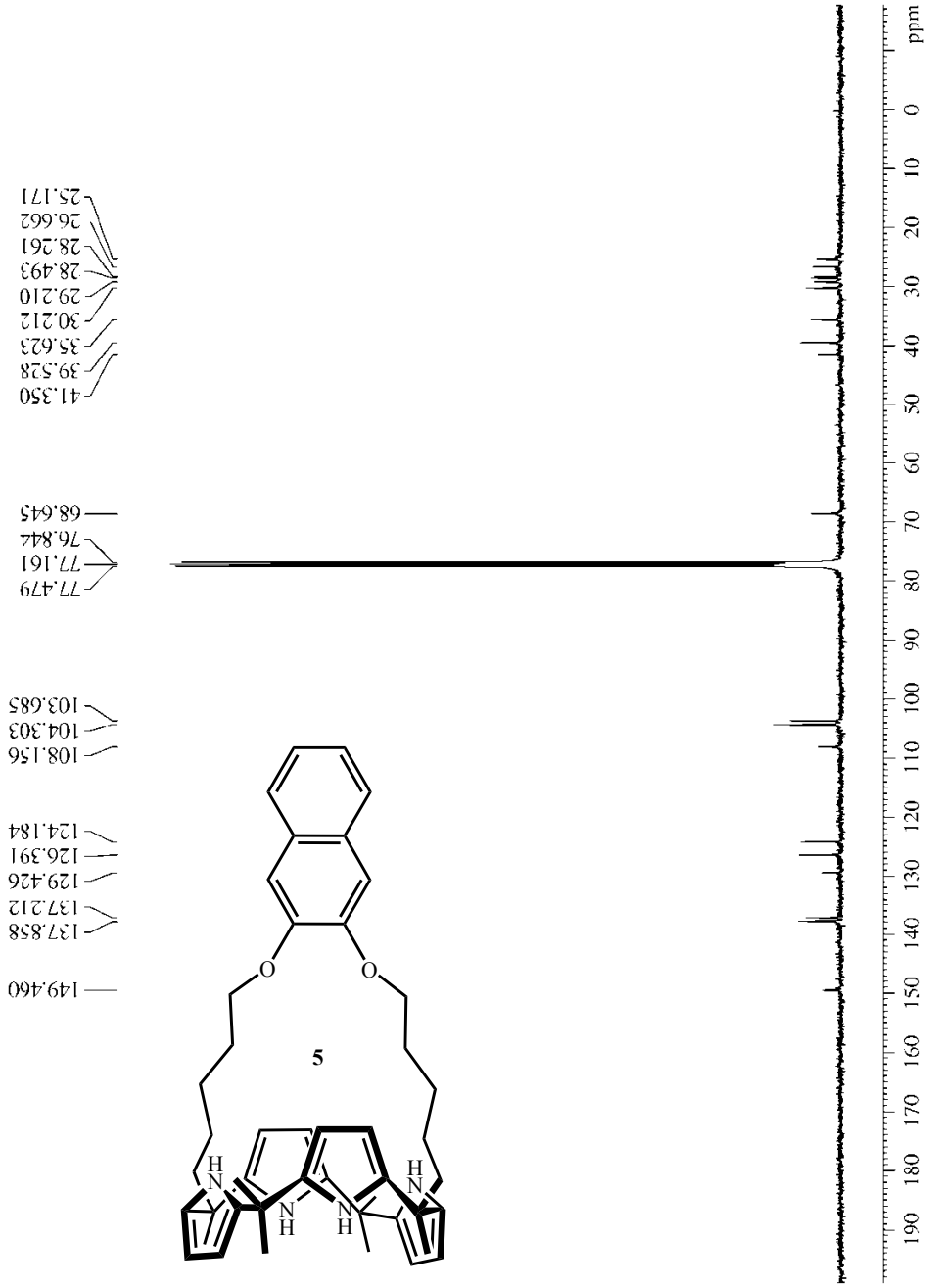


Fig S6:[13]CNMR of Compound **5** in $CDCl_3$.

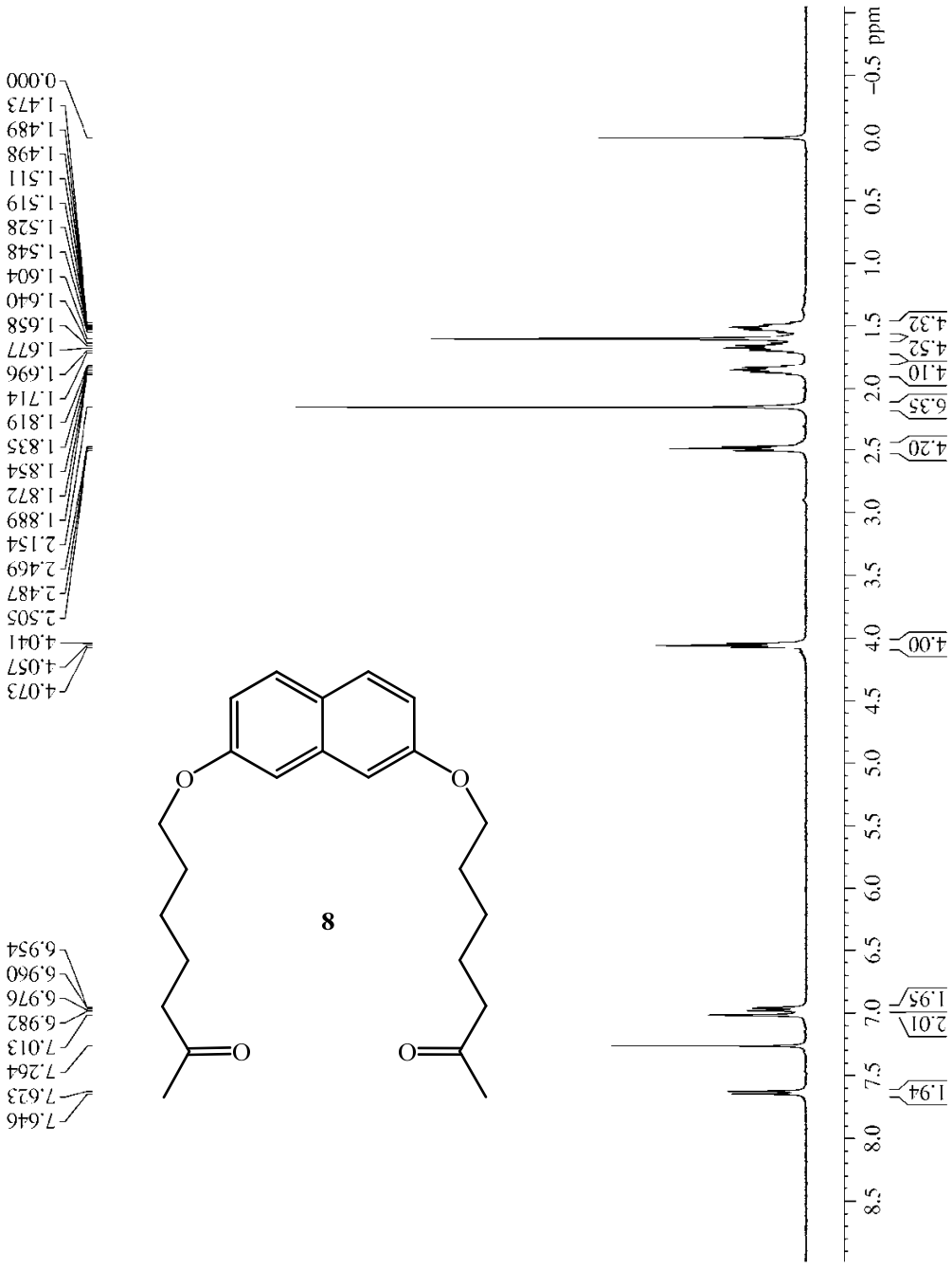


Fig S7:[1]HNMR of Compound **8** in $CDCl_3$.

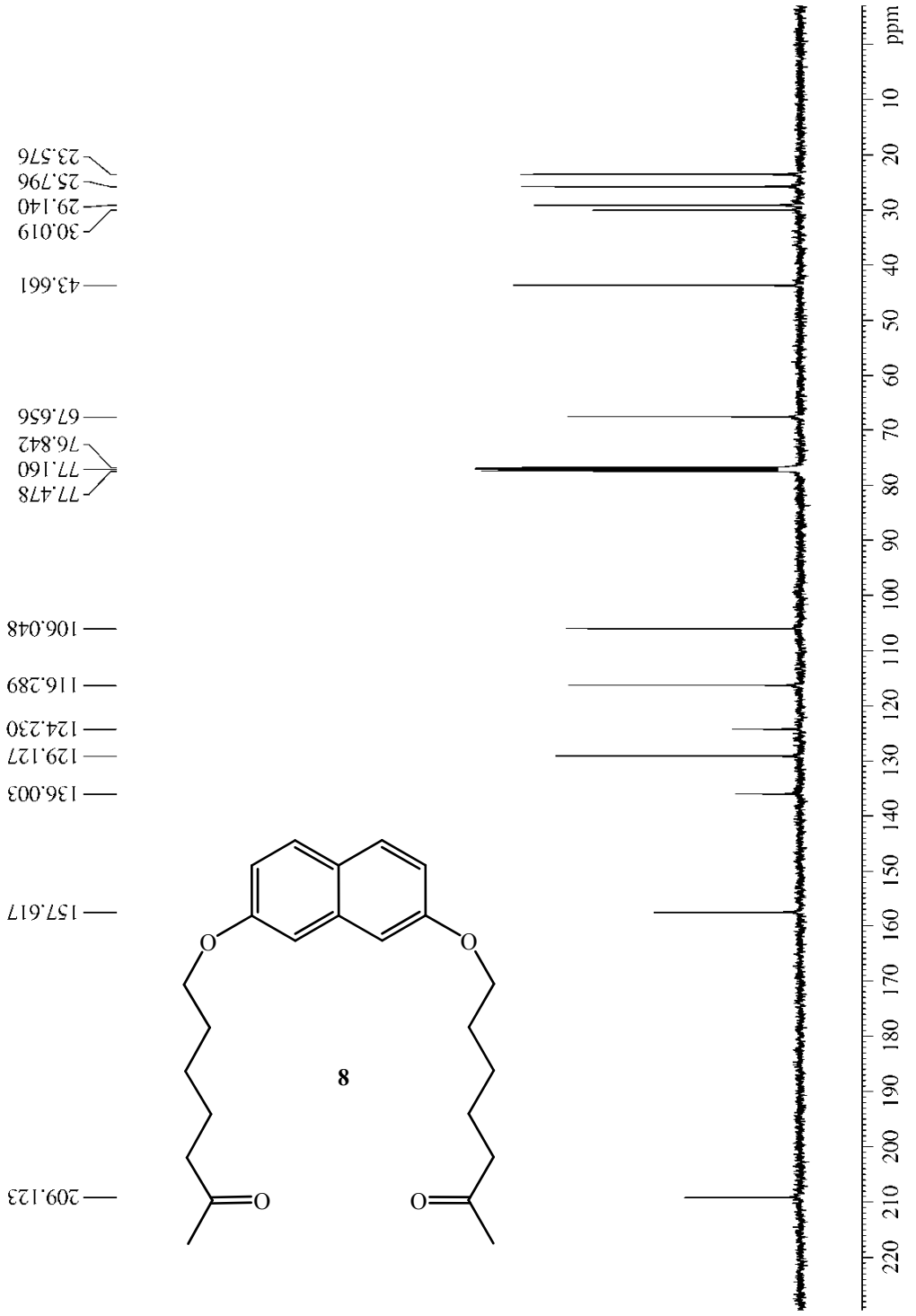


Fig S8:[13]CNMR of Compound **8** in $CDCl_3$.

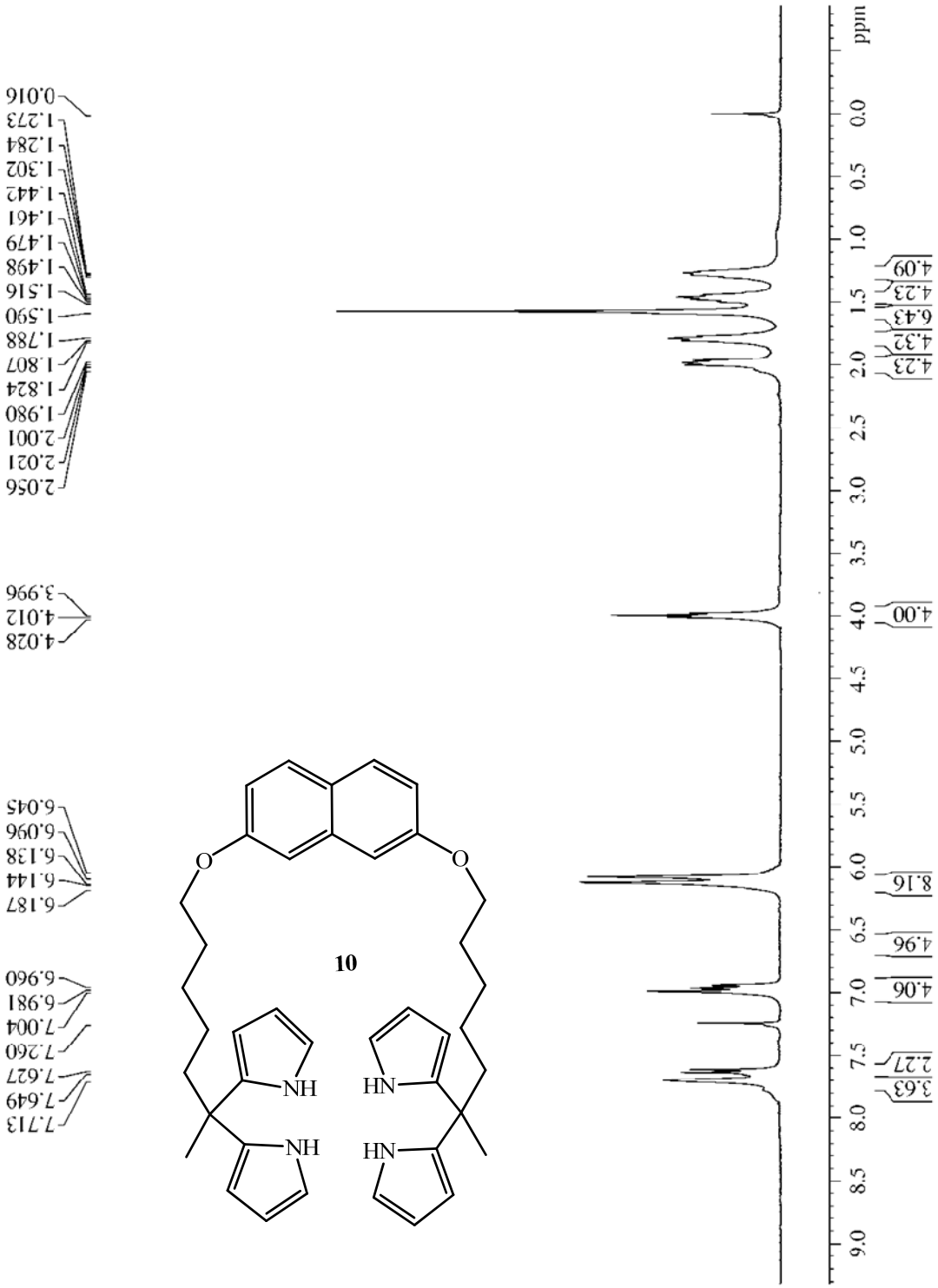


Fig S9:[1]HNMR of Compound **10** in $CDCl_3$.

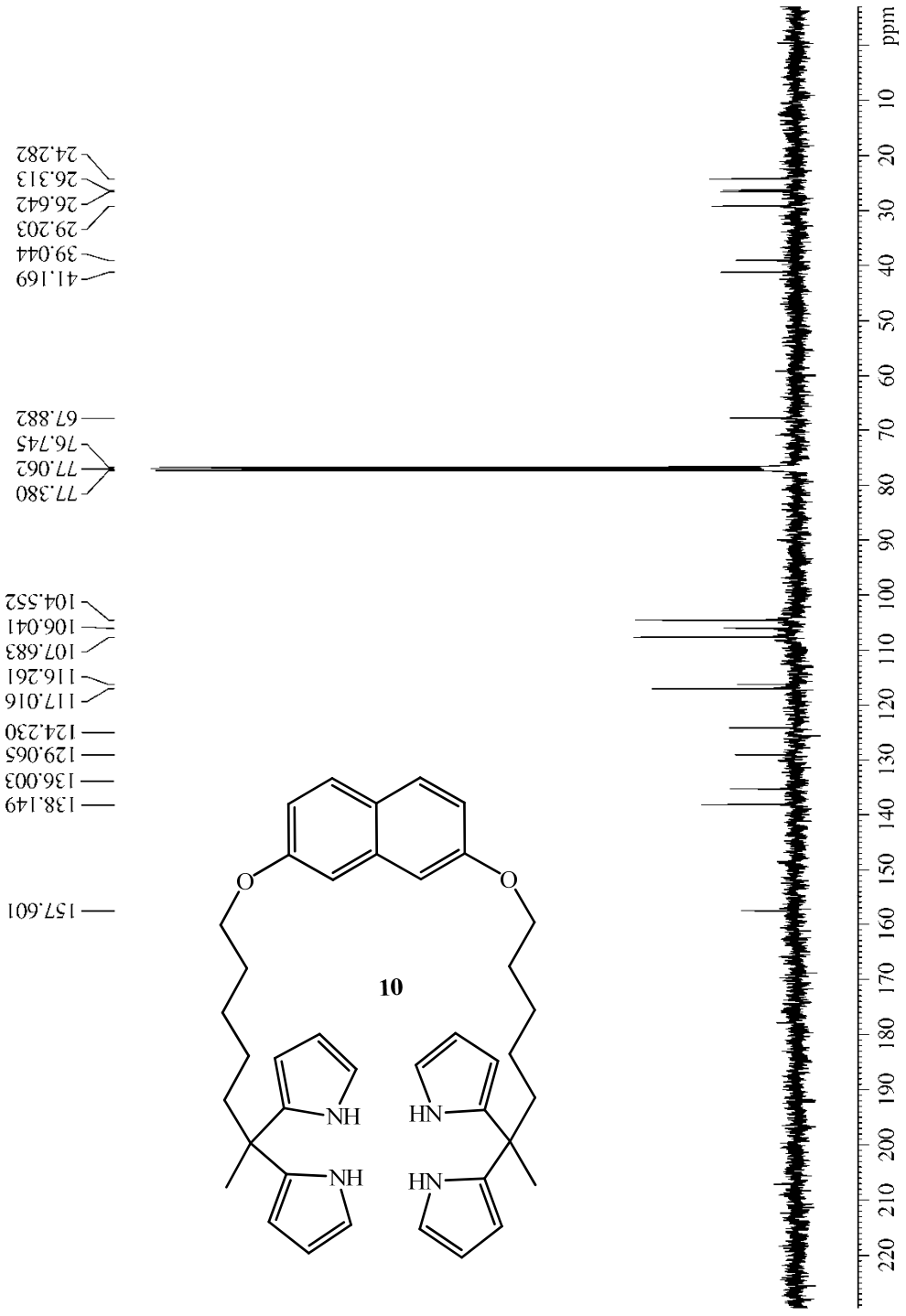


Fig S10:[13]CNMR of Compound **10** in $CDCl_3$.

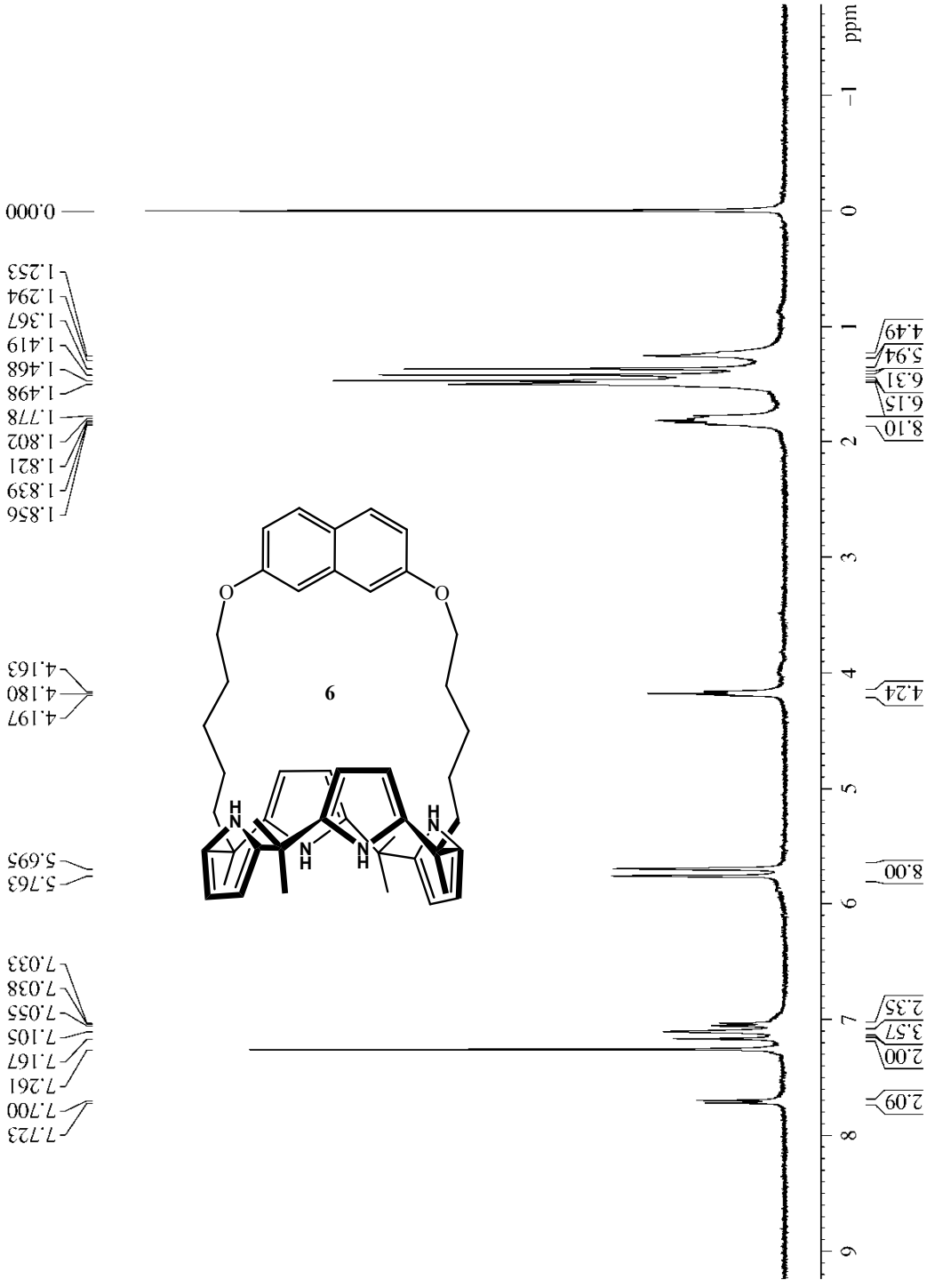


Fig S11:[1]HNMR of Compound **6** in $CDCl_3$.

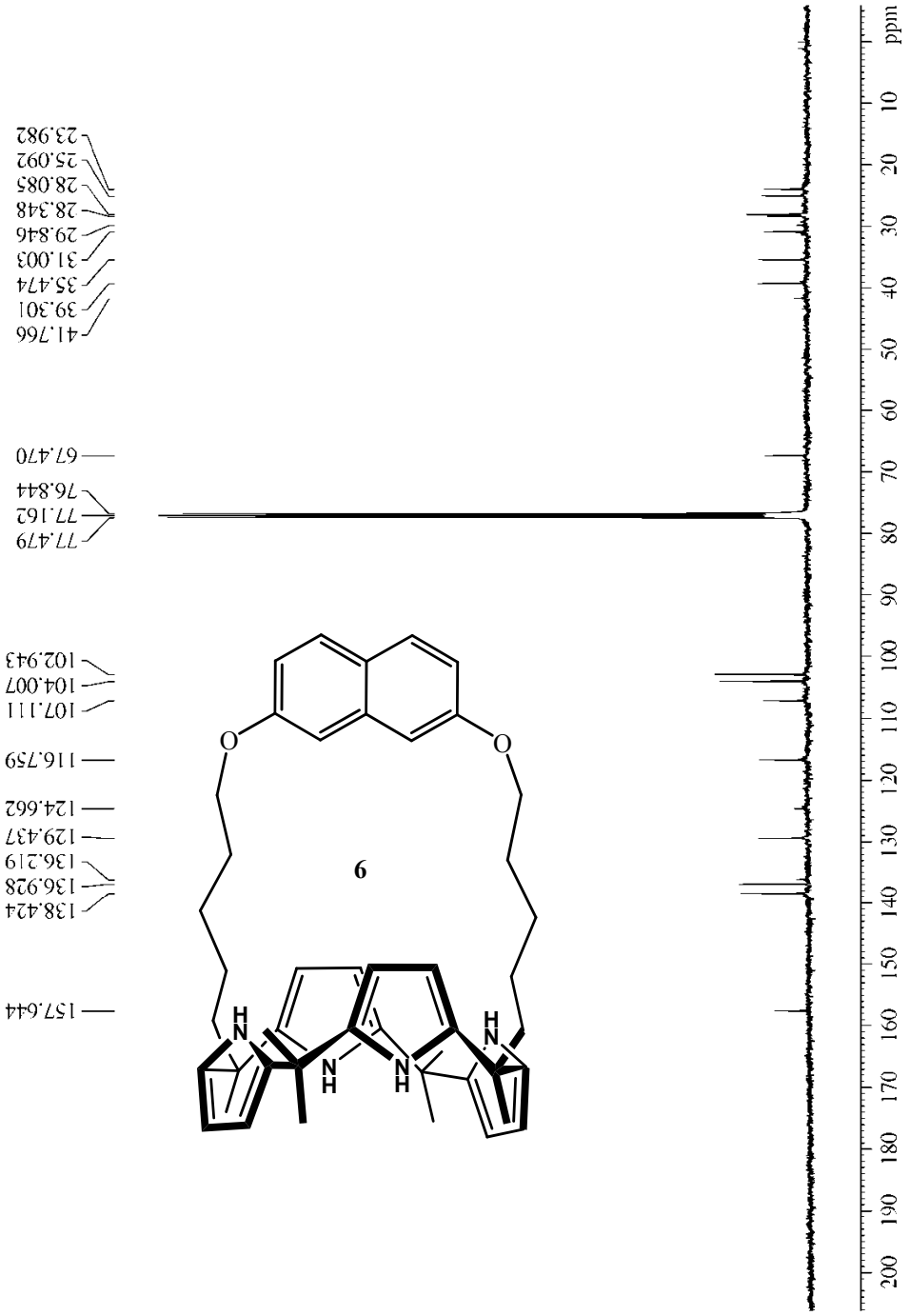


Fig S12:[13]CNMR of Compound **6** in $CDCl_3$.

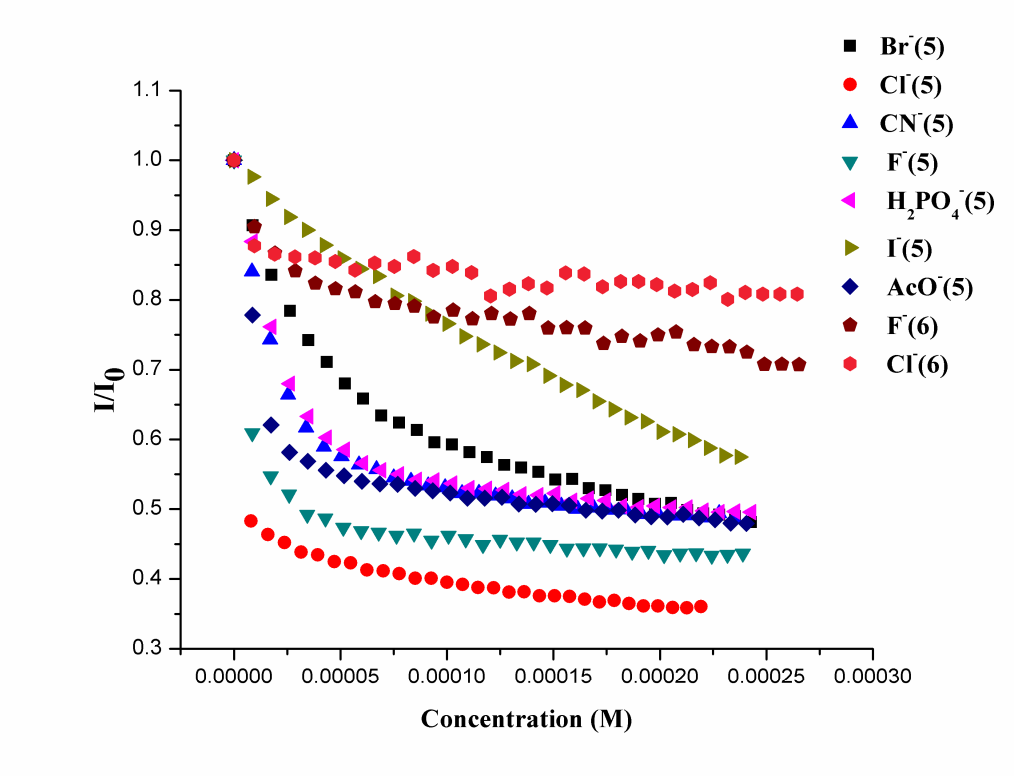


Fig S13: The quenching effect of various anions on compounds **5** and **6**.

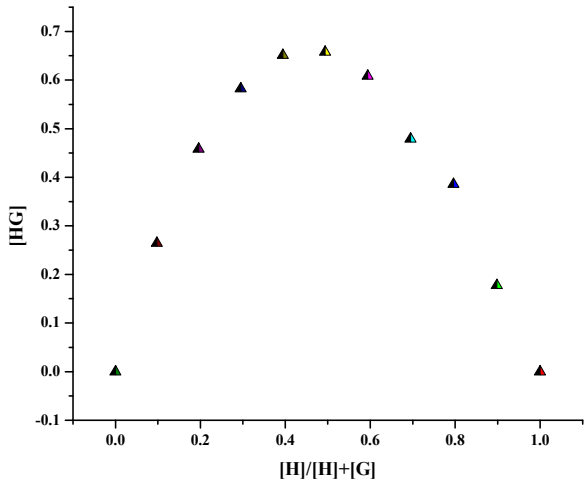


Fig S14: Job plot between compound **5** and tetrabutylammoniumfluoride (TBAF) by fluorescence. The complex concentration, [HG] was calculated by the equation $[HG] = (\Delta I/I_0)\cdot[H]$.

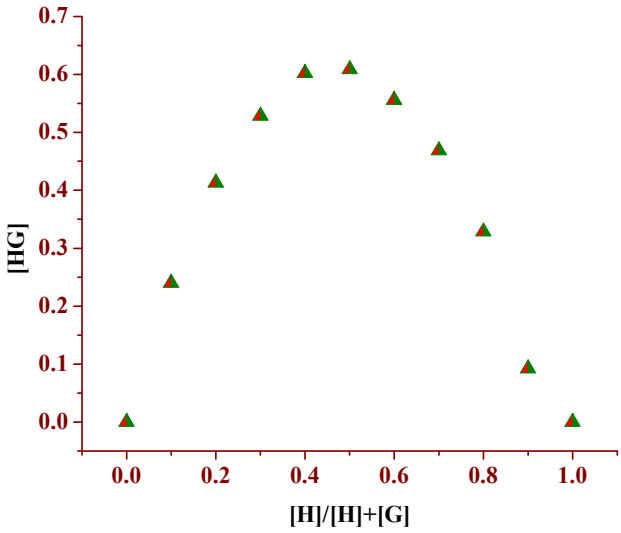


Fig S15: Job plot between compound **5** and tetrabutylammoniumchloride (TBACl) by fluorescence. The complex concentration, [HG] was calculated by the equation $[HG] = (\Delta I/I_0)\cdot[H]$.

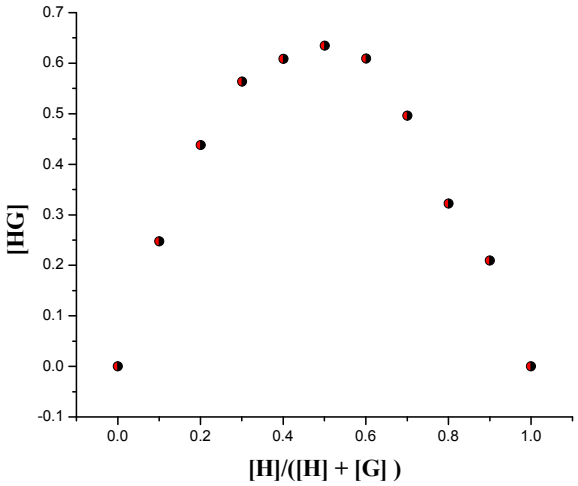


Fig S16: Job plot between compound **6** and tetrabutylammoniumfluoride (TBAF) by fluorescence. The complex concentration, [HG] was calculated by the equation $[HG] = (\Delta I/I_0)\cdot[H]$.

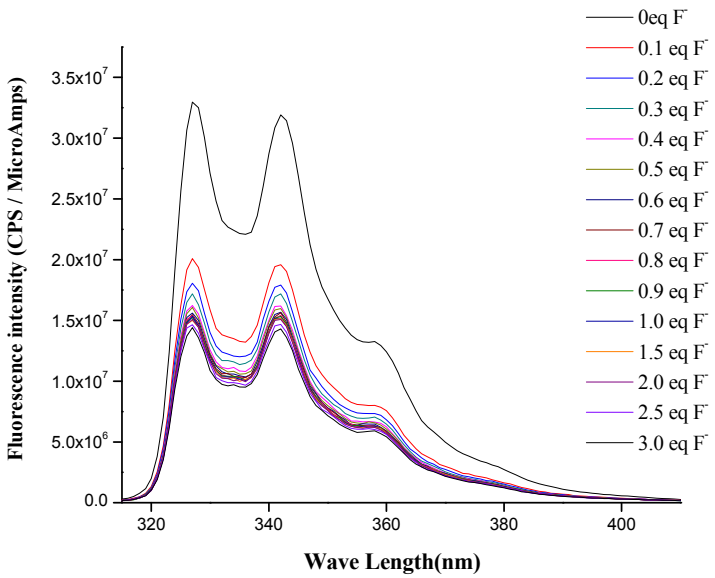


Fig S17: Fluorescence spectra of **5** in CH_3CN (0.0276mM) excited at 310 nm showing the changes induced upon the addition of increasing quantities of tetrabutylammonium fluoride (TBAF).

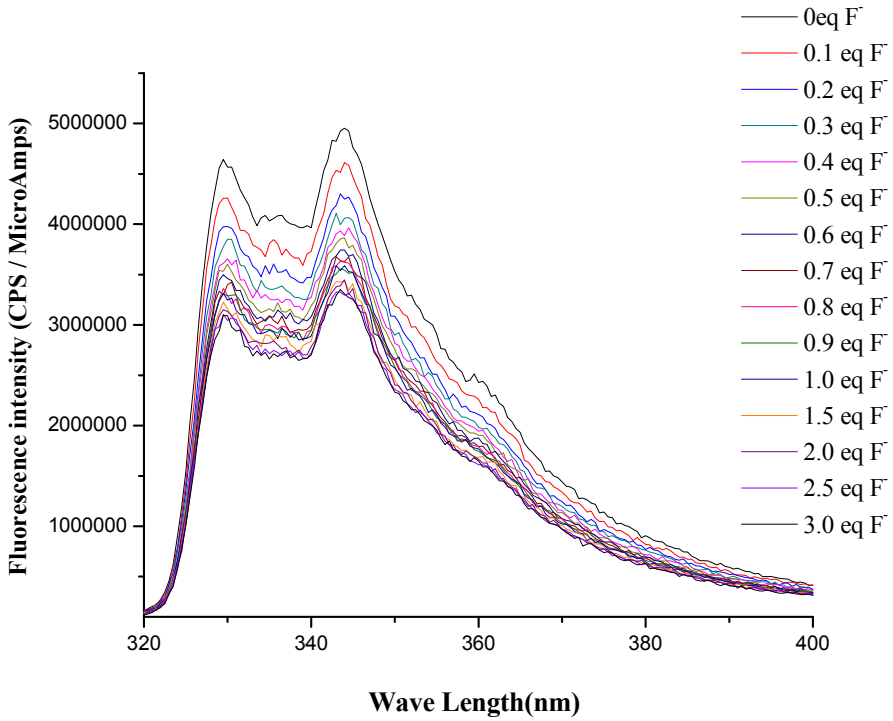


Fig S18:Fluorescence spectra of **6** in CH_3CN (0.0305mM) excited at 316 nm showing the changes induced upon the addition of increasing quantities of tetrabutylammonium fluoride (TBAF).

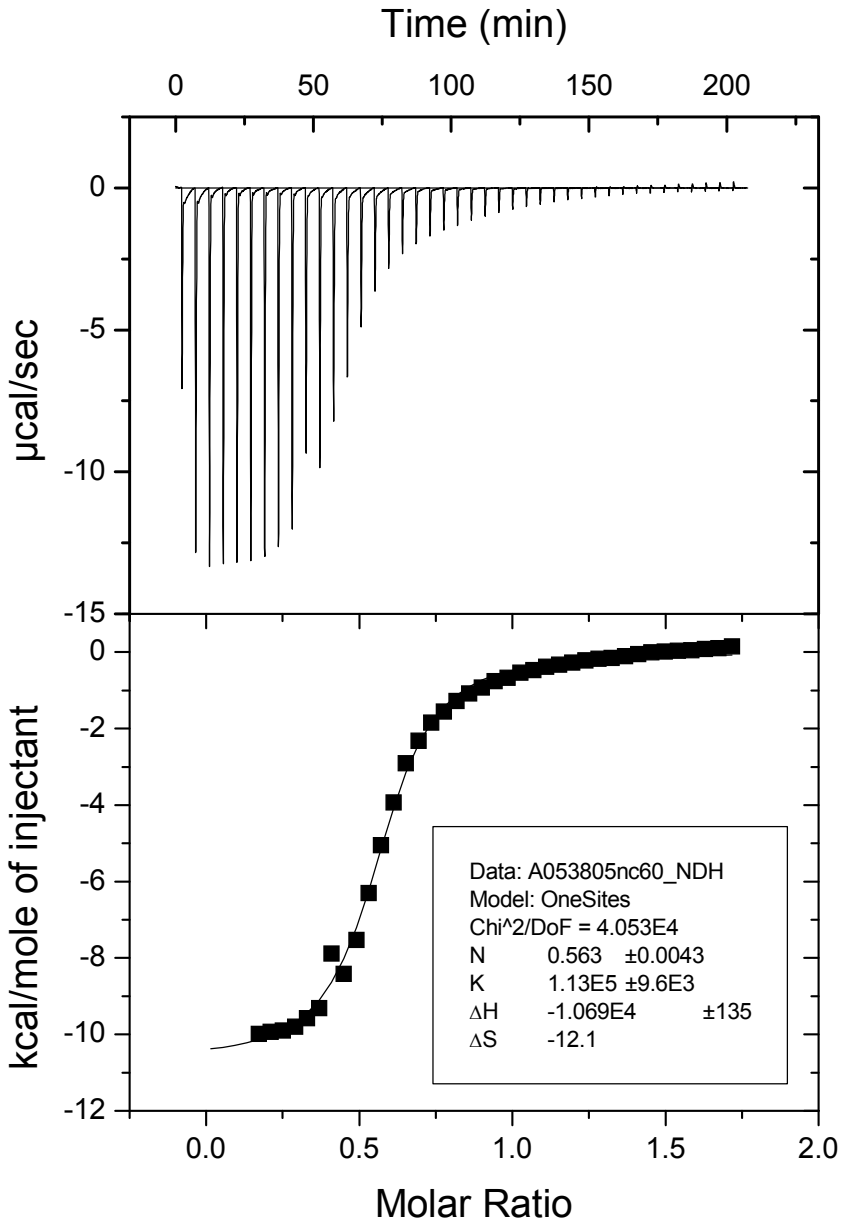


Fig S19: Isothermal calorimetric titration in acetonitrile at 303 K of tetrabutylammonium acetate (0.058 M) added into the solution of **5** at 3.05 mM. The curve shows the fit of the experimental data to a 1:1 binding profile.

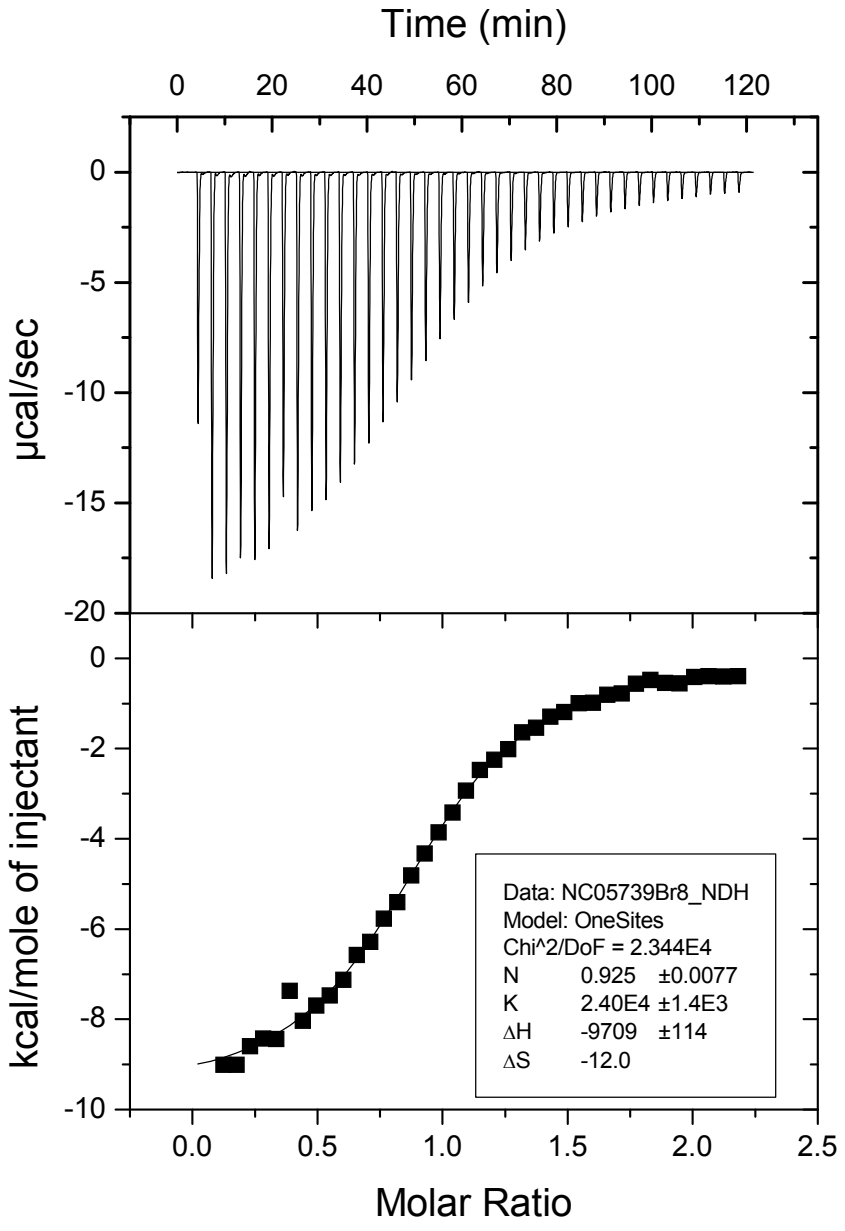


Fig S20: Isothermal calorimetric titration in acetonitrile at 303 K of tetrabutylammonium bromide (0.057 M) added into the solution of **5** at 3.05 mM. The curve shows the fit of the experimental data to a 1:1 binding profile.

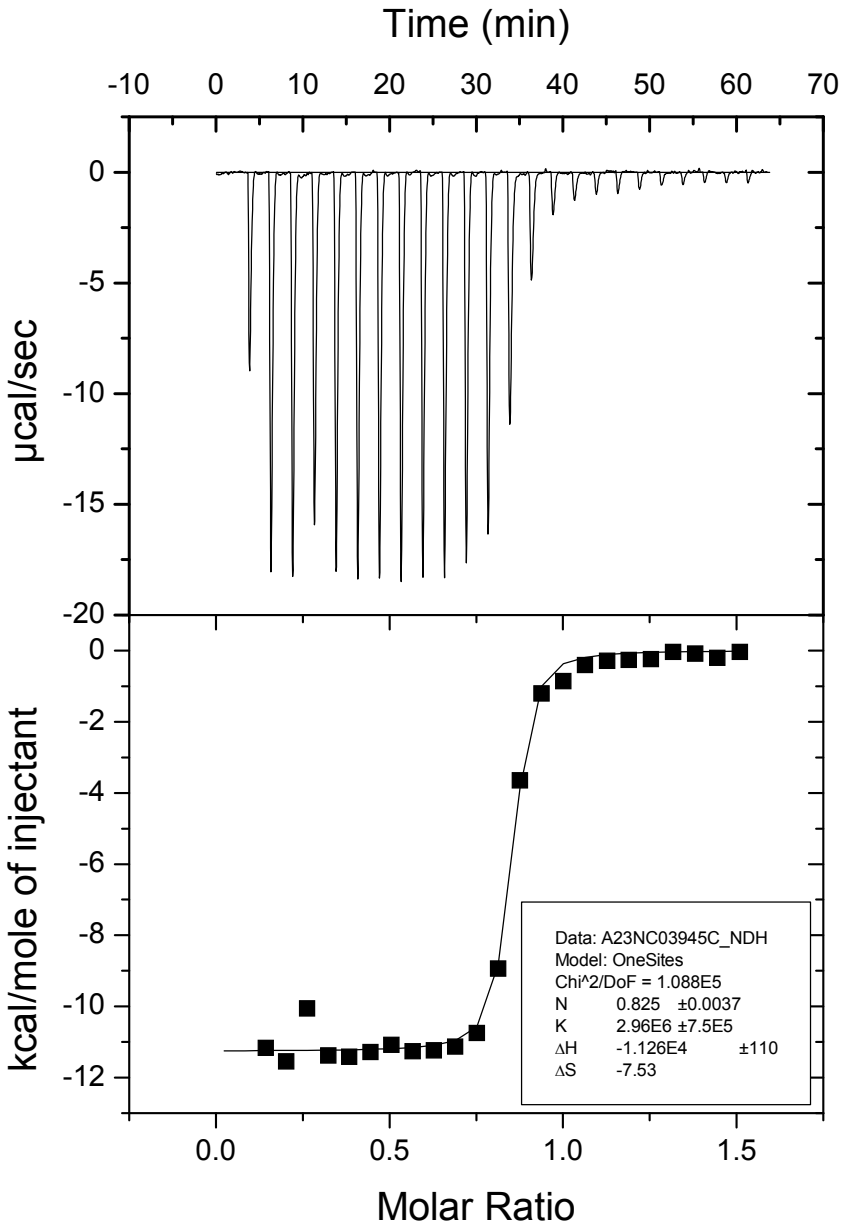


Fig S21: Isothermal calorimetric titration in acetonitrile at 303 K of tetrabutylammonium chloride (0.035 M) added into the solution of **5** at 0.57 mM. The curve shows the fit of the experimental data to a 1:1 binding profile.

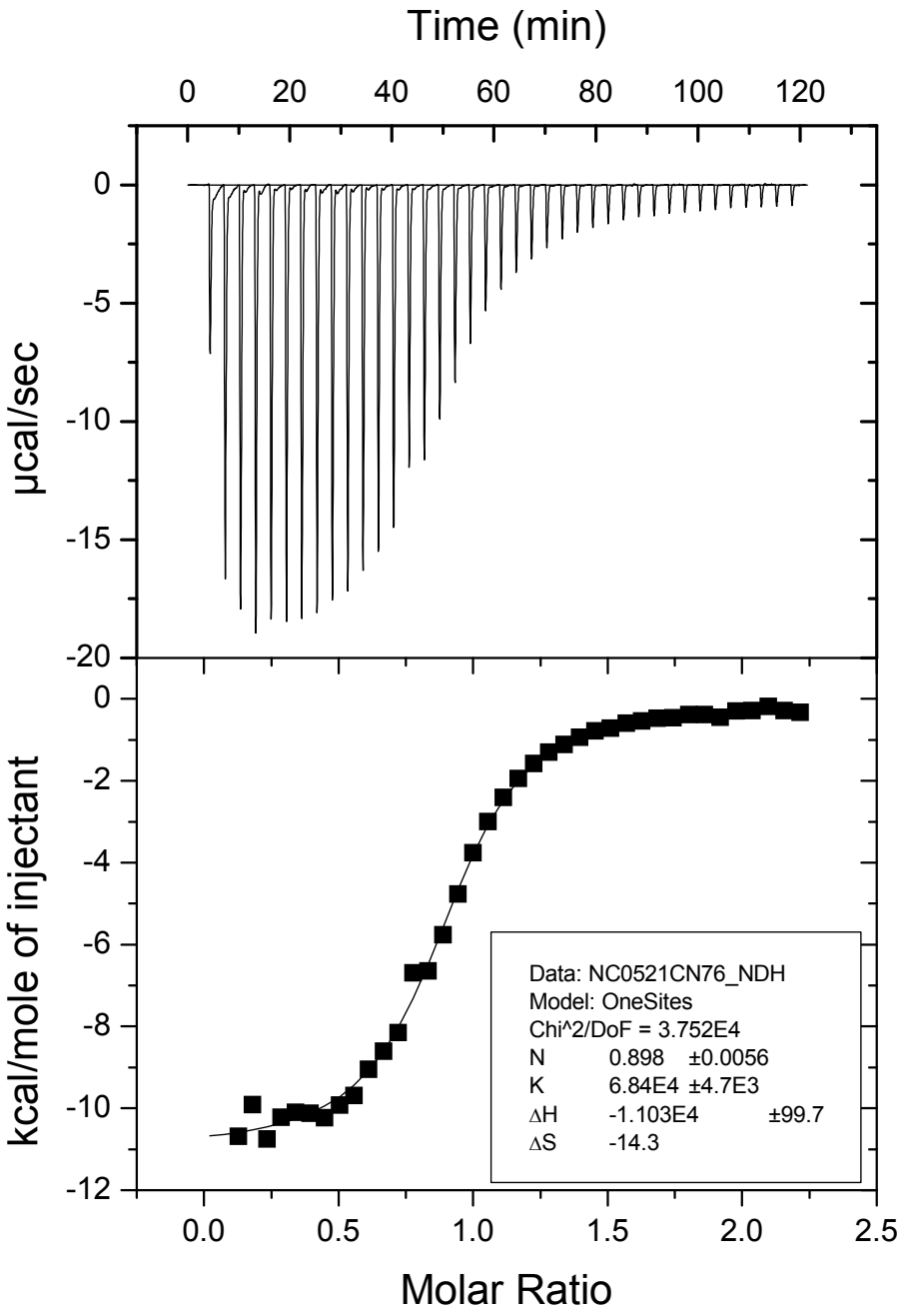


Fig S22: Isothermal calorimetric titration in acetonitrile at 303 K of tetrabutylammonium cyanide (0.052 M) added into the solution of **5** at 0.7 mM. The curve shows the fit of the experimental data to a 1:1 binding profile.

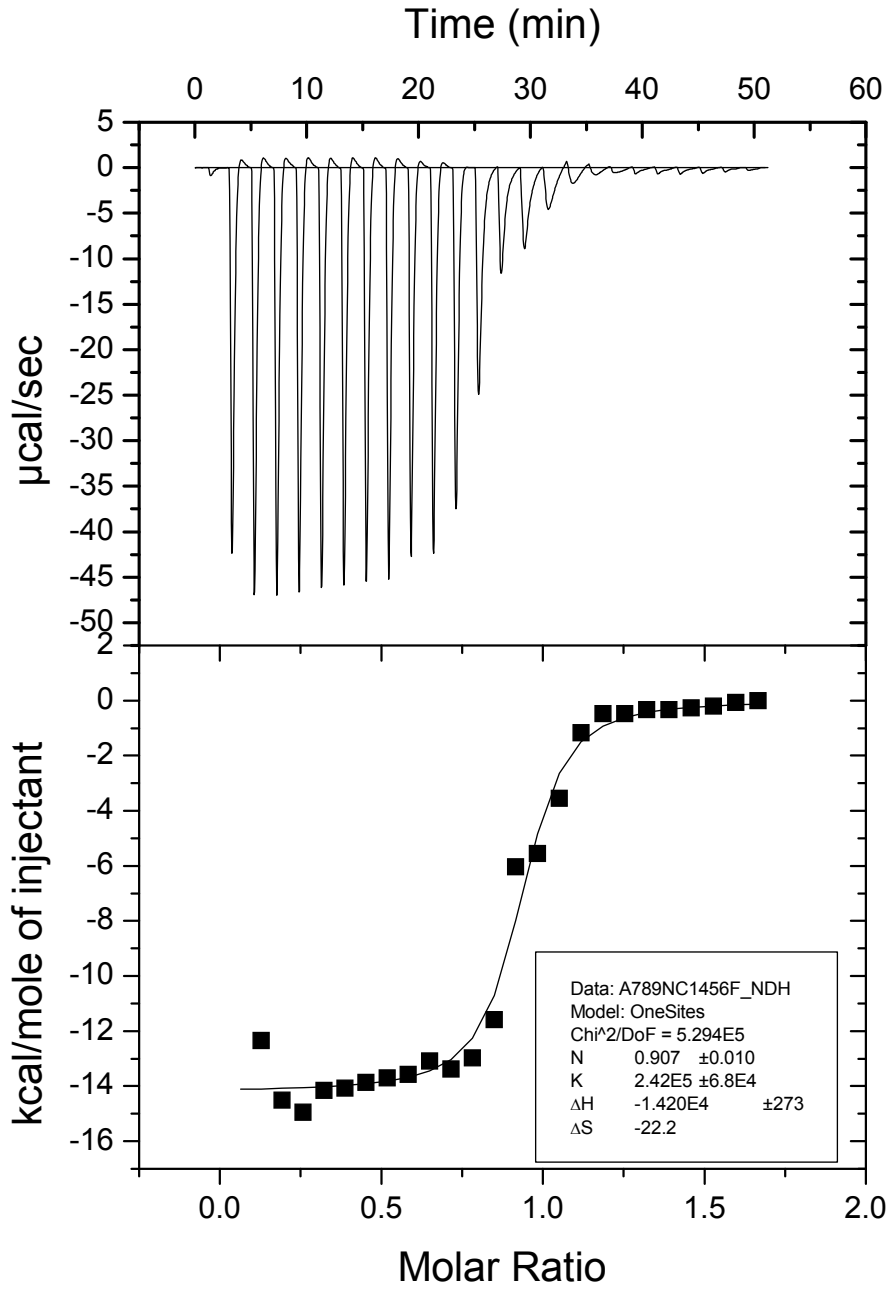


Fig S23: Isothermal calorimetric titration in acetonitrile at 303 K of tetrabutylammonium fluoride (0.99 M) added into the solution of **5** at 0.789 mM. The curve shows the fit of the experimental data to a 1:1 binding profile.

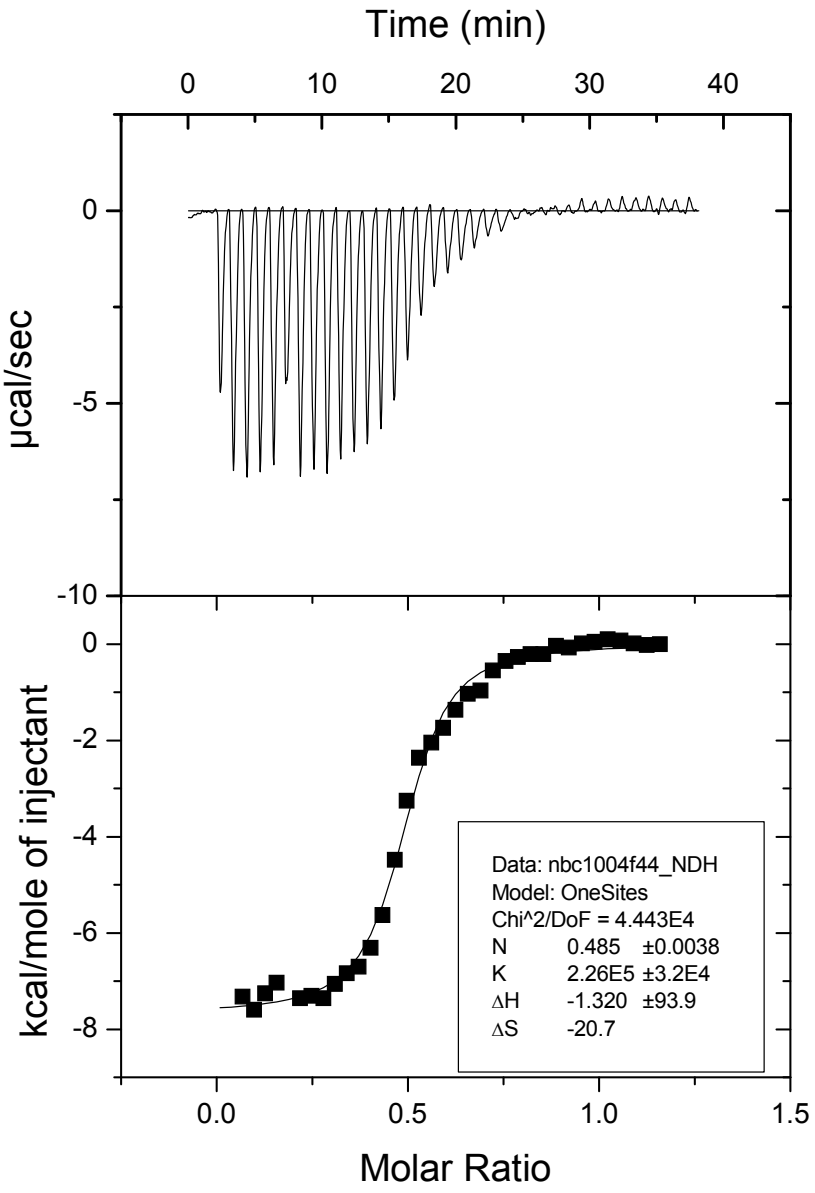


Fig S24: Isothermal calorimetric titration in acetonitrile at 303 K of tetrabutylammonium fluoride (0.99 M) added into the solution of **5** at 0.789 mM (measurement was carried out in 0.5% water-acetonitrile).

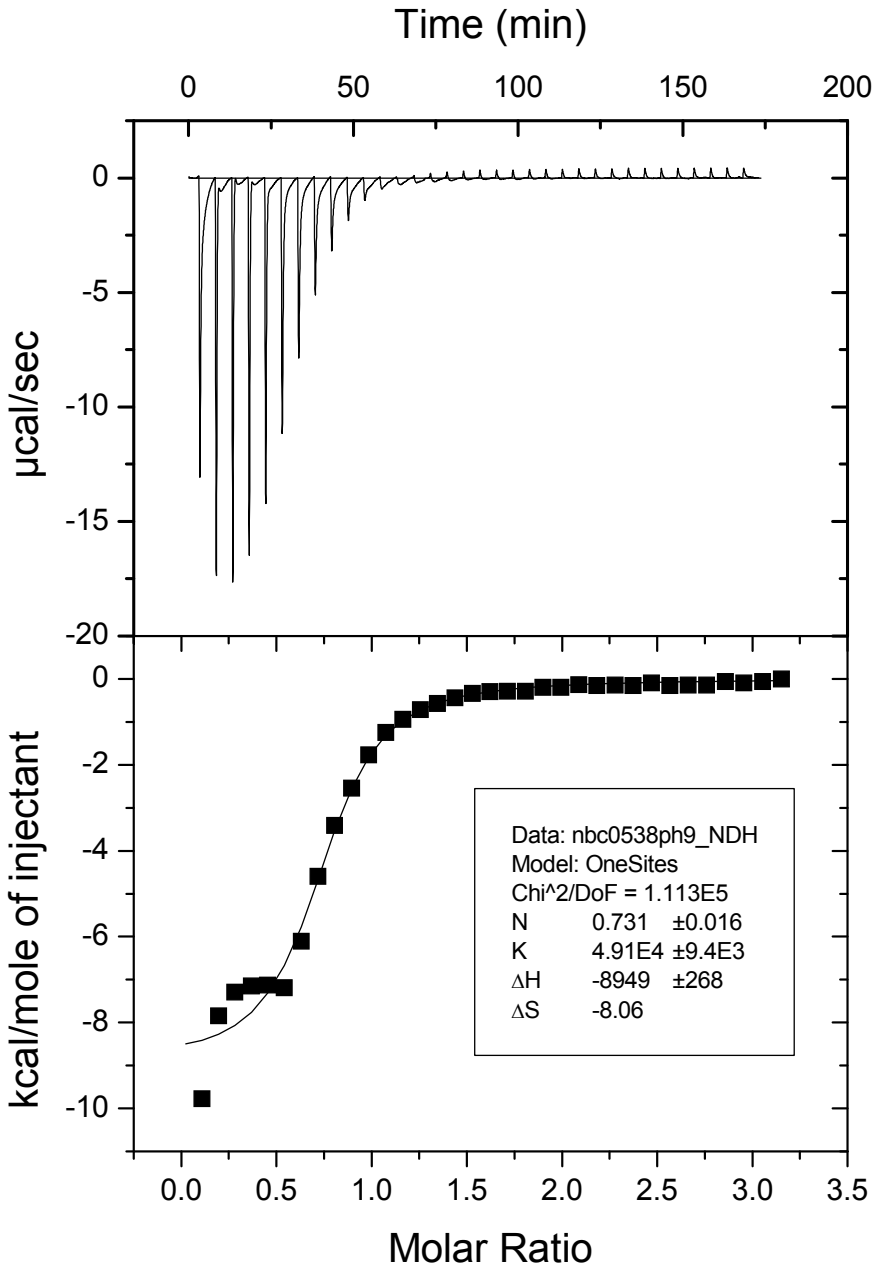


Fig S25: Isothermal calorimetric titration in acetonitrile at 303 K of tetrabutylammonium dihydrogenphosphate (0.064 M) added into the solution of **5** at 0.57 mM. The curve shows the fit of the experimental data to a 1:1 binding profile.

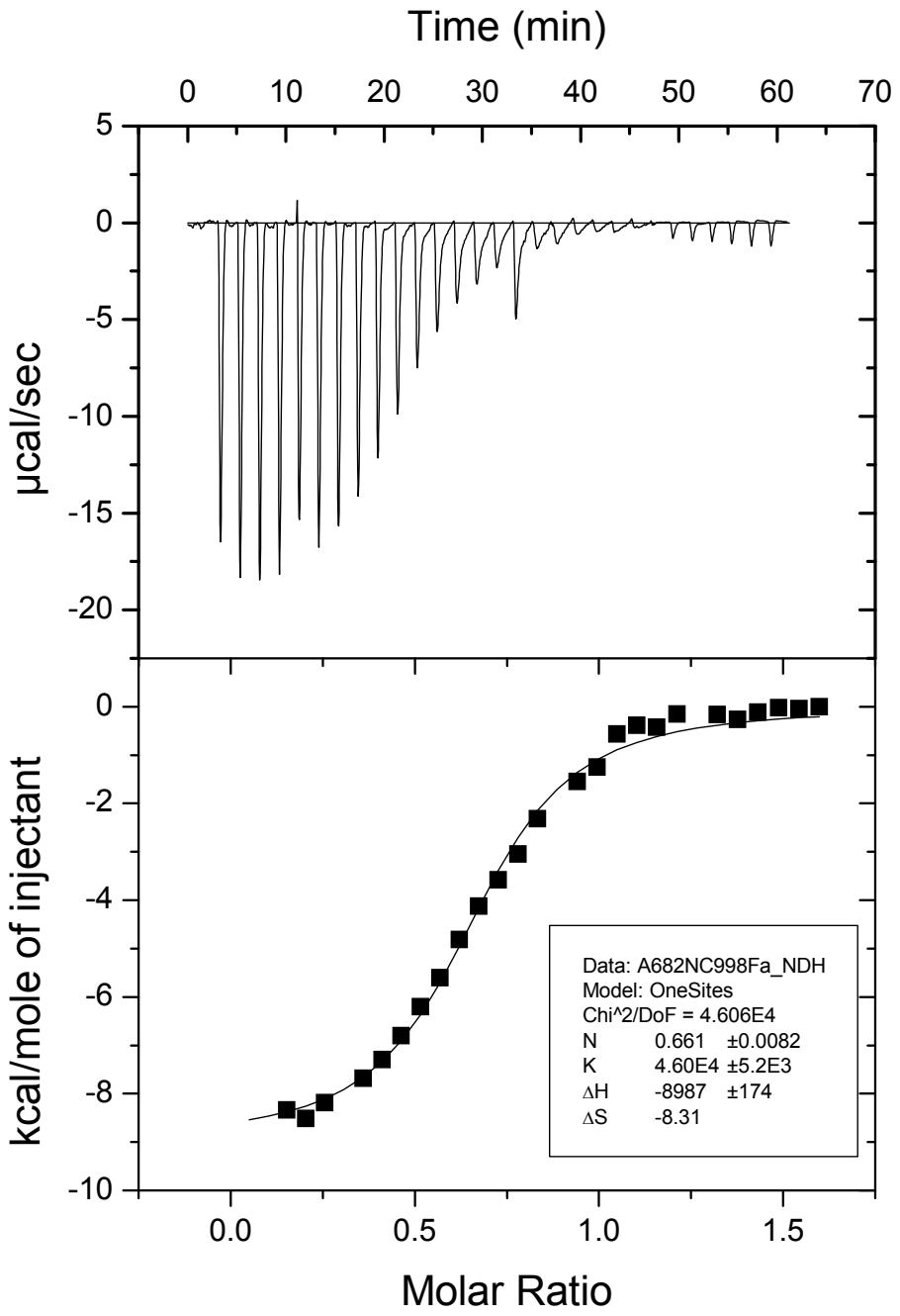


Fig S26: Isothermal calorimetric titration in acetonitrile at 303 K of tetrabutylammonium fluoride (0.998 M) added into the solution of **6** at 0.68 mM. The curve shows the fit of the experimental data to a 1:1 binding profile.

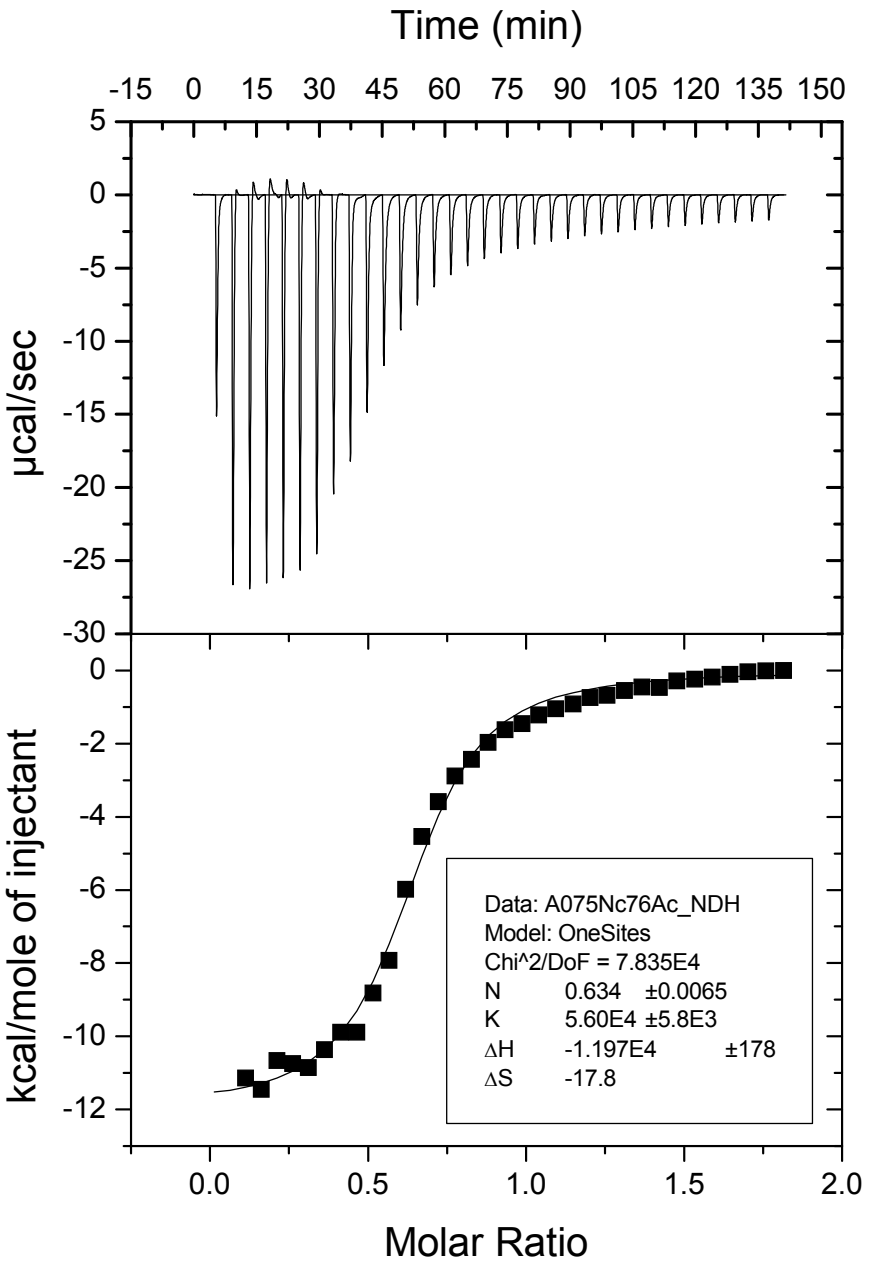


Fig S27: Isothermal calorimetric titration in acetonitrile at 303 K of tetrabutylammonium acetate (0.760 M) added into the solution of **6** at 0.75mM. The curve shows the fit of the experimental data to a 1:1 binding profile.

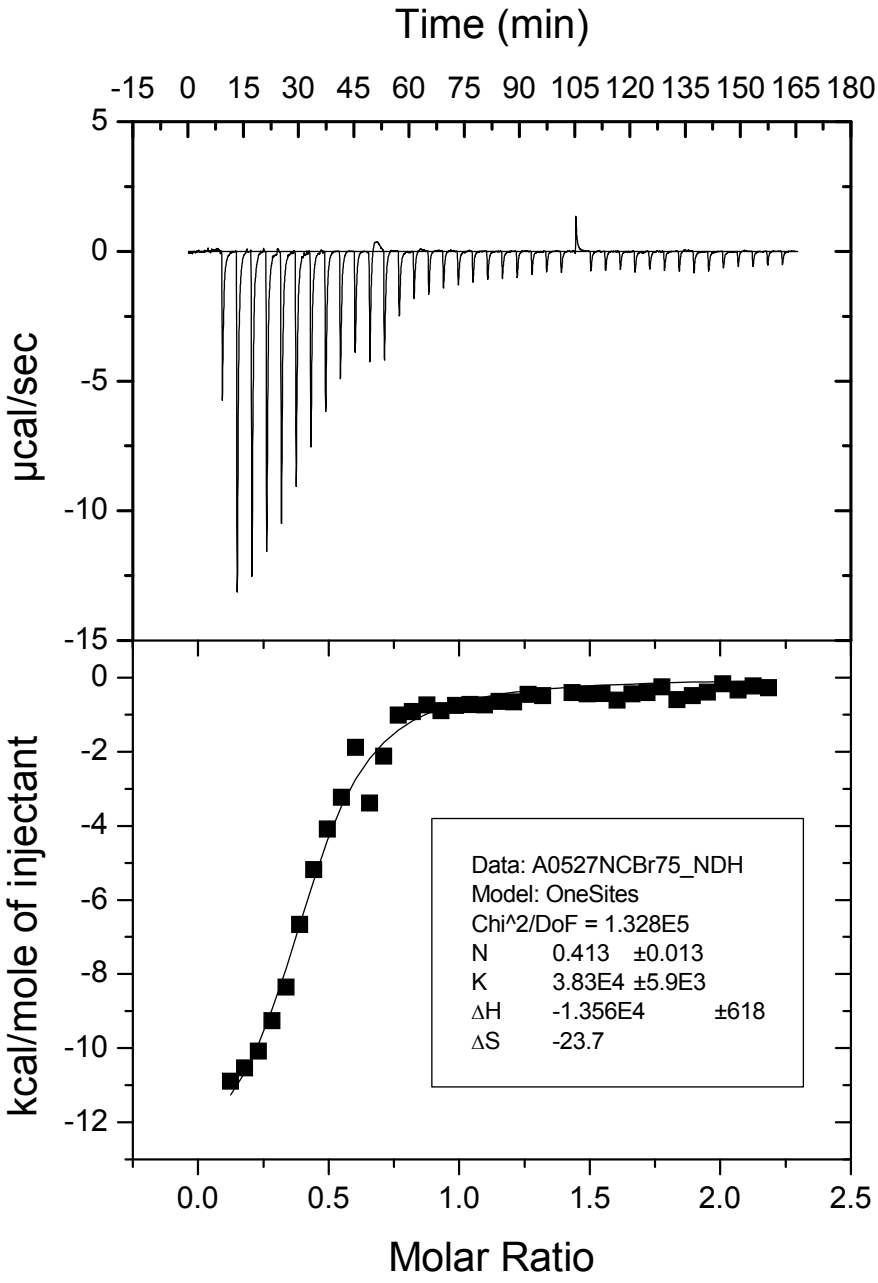


Fig S28: Isothermal calorimetric titration in acetonitrile at 303 K of tetrabutylammonium bromide (0.75 M) added into the solution of **6** at 0.57mM. The curve shows the fit of the experimental data to a 1:1 binding profile.

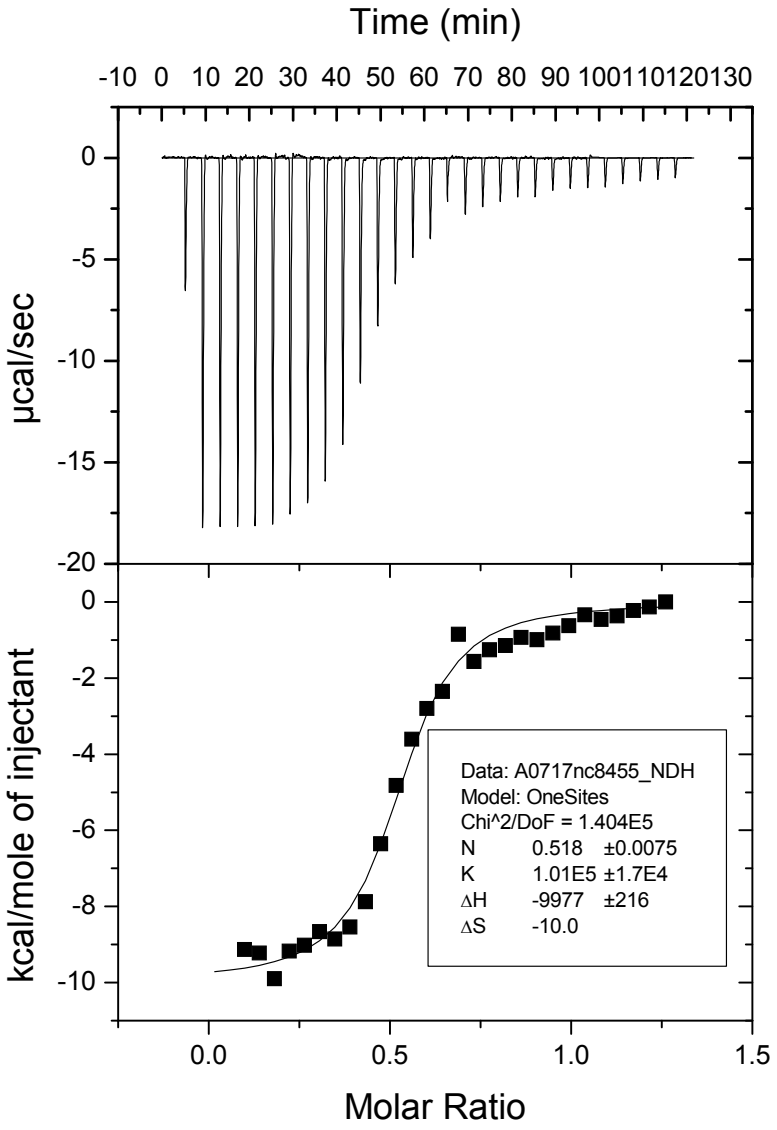


Fig S29: Isothermal calorimetric titration in acetonitrile at 303 K of tetrabutylammonium chloride (0.85 M) added into the solution of **6** at 0.717mM. The curve shows the fit of the experimental data to a 1:1 binding profile.

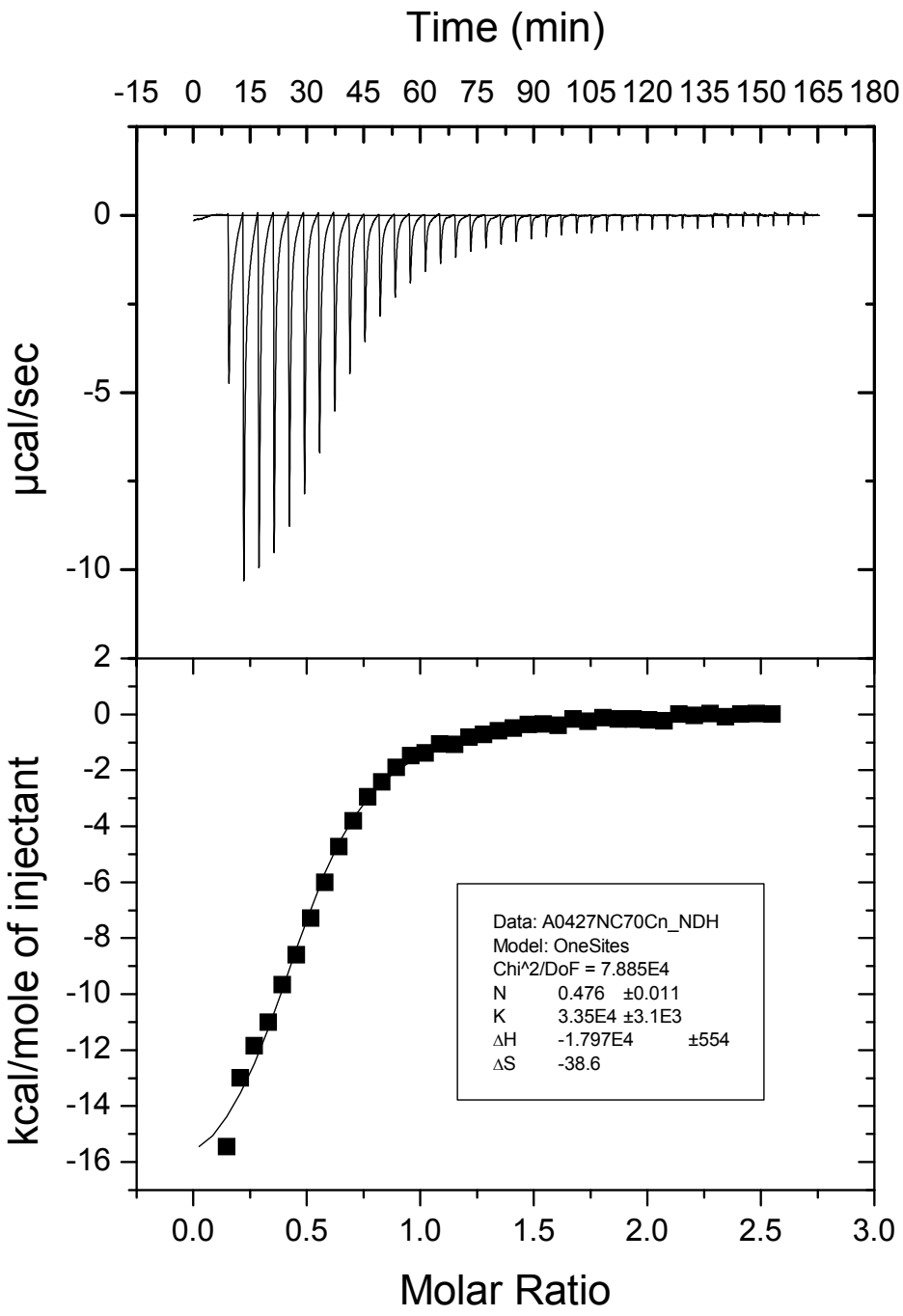


Fig S30: Isothermal calorimetric titration in acetonitrile at 303 K of tetrabutylammonium cyanide (0.70 M) added into the solution of **6** at 0.43mM. The curve shows the fit of the experimental data to a 1:1 binding profile.

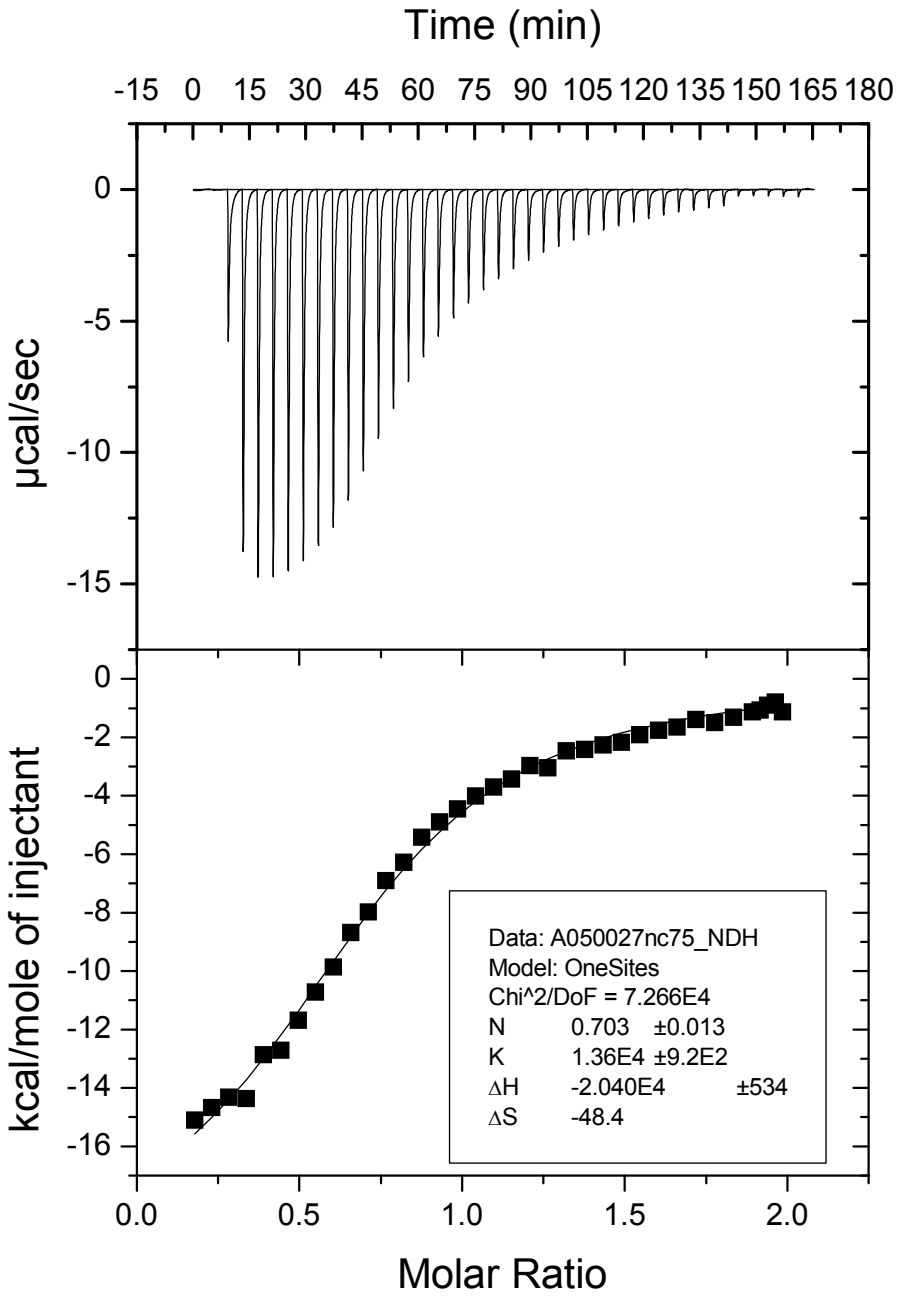


Fig S31: Isothermal calorimetric titration in acetonitrile at 303 K of tetrabutylammonium dihydrogenphosphate (0.75 M) added into the solution of **6** at 0.50mM. The curve shows the fit of the experimental data to a 1:1 binding profile.

Table 1: Association constants (K_a, M^{-1}) for the interaction of receptors with different anions in acetonitrile at 303K.

Anion	4[(a), (b)]	5[(c)]	5[(a)]	6[(c)]	6[(a)]
F^-	- 1.17×10^{6}[(d)]	2.42×10^{5} -	2.42×10^{5} 2.26×10^{5}[(d)]	4.20×10^{4} -	4.60×10^{4} -
Cl^-	2.12×10^{6}	2.28×10^{6}	2.96×10^{6}	7.20×10^{2}	1.01×10^{5}
Br^-	1.95×10^{6}	2.92×10^{4}	2.40×10^{4}	[e]	3.38×10^{4}
CN^-	[f]	6.31×10^{4}	6.84×10^{4}	[e]	3.35×10^{4}
$H_2PO_4^-$	1.07×10^{5}	5.30×10^{4}	4.91×10^{4}	[e]	1.36×10^{4}
CH_3COO^-	1.28×10^{5}	1.21×10^{5}	1.13×10^{5}	[e]	5.6×10^{4}

Note: [a] determined by ITC; [b] data from ref. S5; [c] determined by fluorescence study; [d] measured in 0.5% water-acetonitrile; [e] binding constants could not be evaluated; [f] not reported.

Table 2: Thermodynamic data derived from isothermal titration calorimetry (ITC) for the Interactions of receptors **5** and **6** with tetrabutylammonium salts at 303K.

Anion	5			6		
	ΔH(kcal/mole)	**TΔS(kcal/mole)**	**ΔG(kcal/mole)**	**ΔH(kcal/mole)**	**TΔS(kcal/mole)**	**ΔG(kcal/mole)**
F^-	-14.20	-6.507	-7.473	-8.987	-2.518	-6.577
Cl^-	-11.26	-2.292	-8.968	-9.977	-3.03	-6.947
Br^-	-9.709	-0.0120	-6.073	-13.56	-7.181	-6.379
CN^-	-11.03	-4.333	-6.697	-17.97	-11.696	-6.274
$H_2PO_4^-$	-8.949	-2.442	-6.507	-20.40	-14.665	-5.735
CH_3COO^-	-10.69	-0.0121	-7.0237	-11.97	-5.393	-6.577

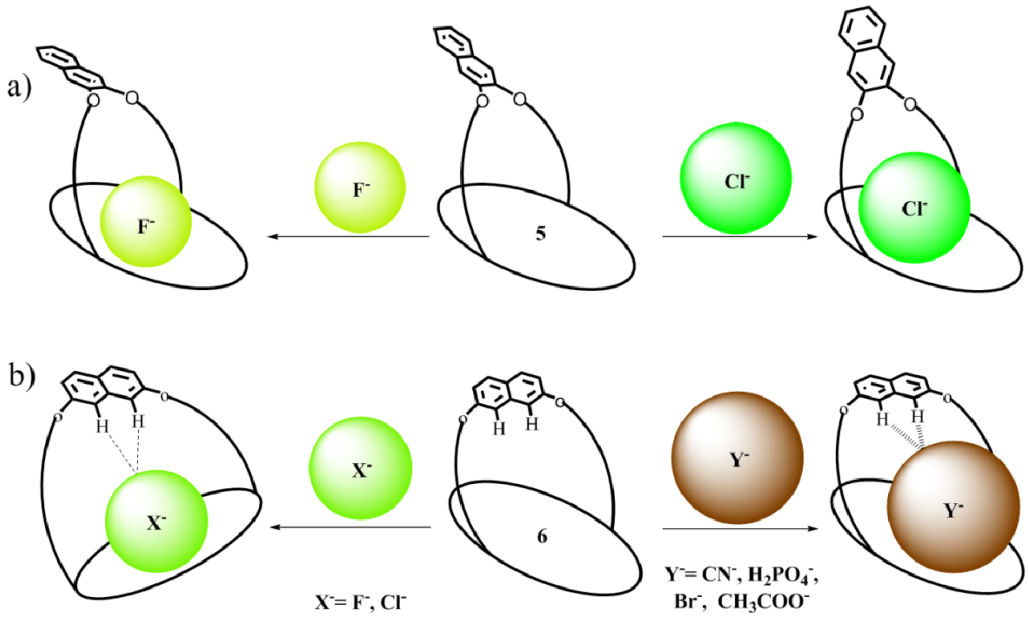


Fig S32: Plausible binding modes of different anions for **5** and **6**.

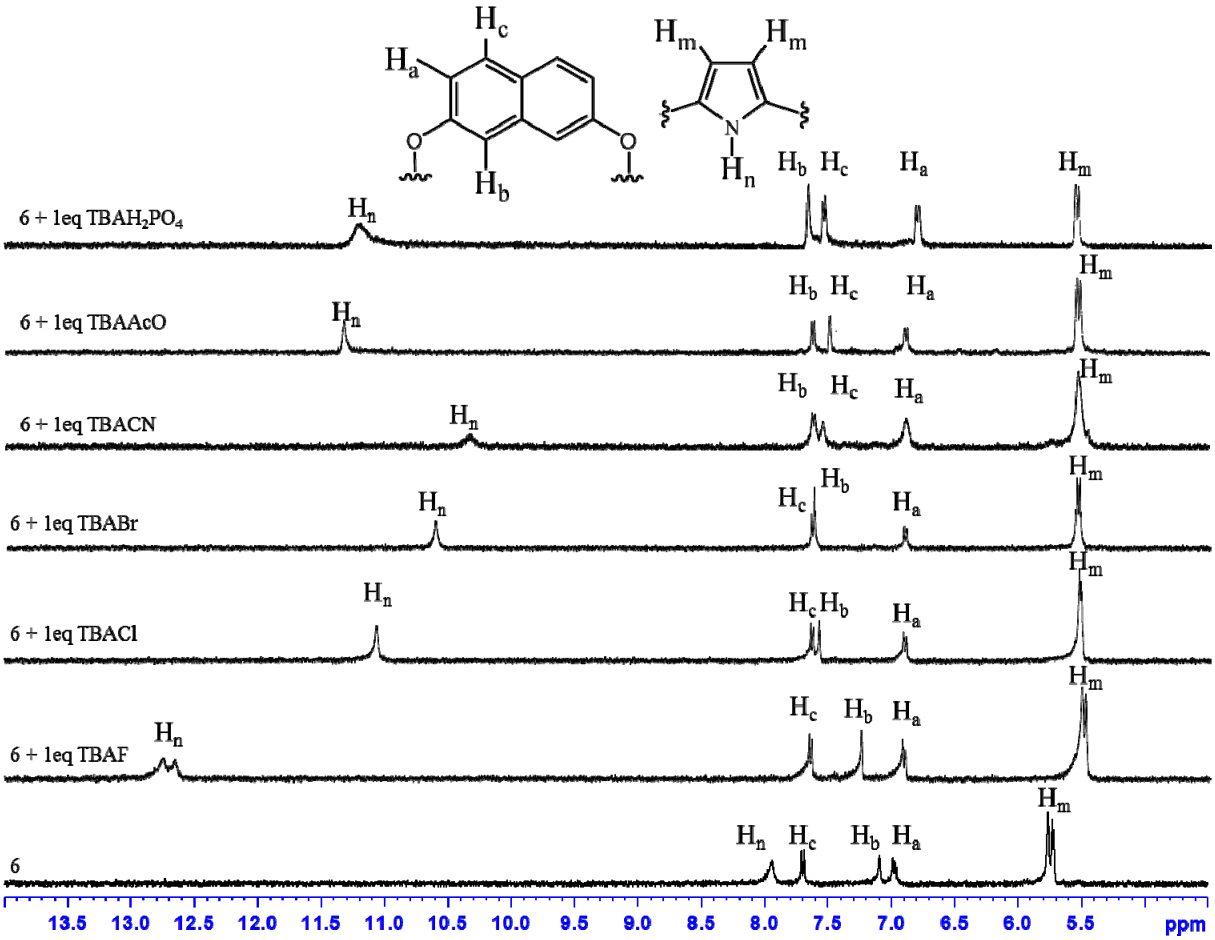


Fig S33: Changes in ^{1}H NMR spectrum of **6** after addition one equivalent of various anions in CD_3CN. (partial ^{1}H-NMR spectrum of **6** shown)

Computational (DFT) analysis:

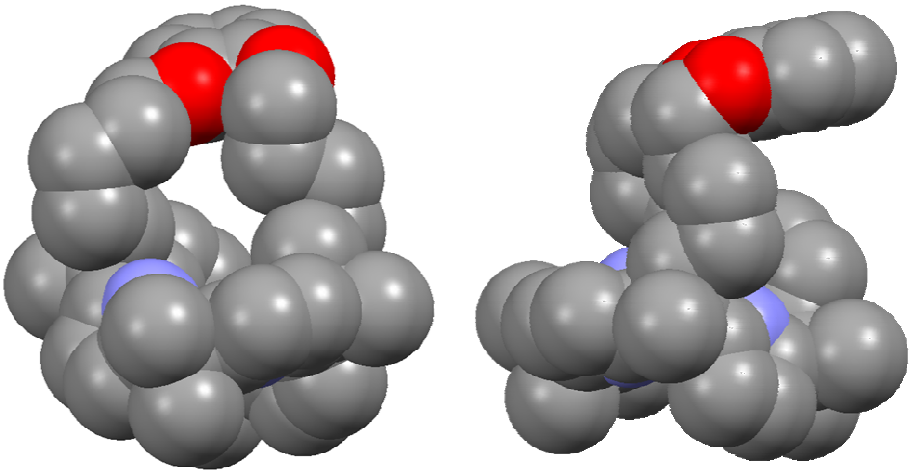


Fig S34: Space-filling model view of DFT optimized structure of **4.** (Hydrogen atoms are removed for clarity.)

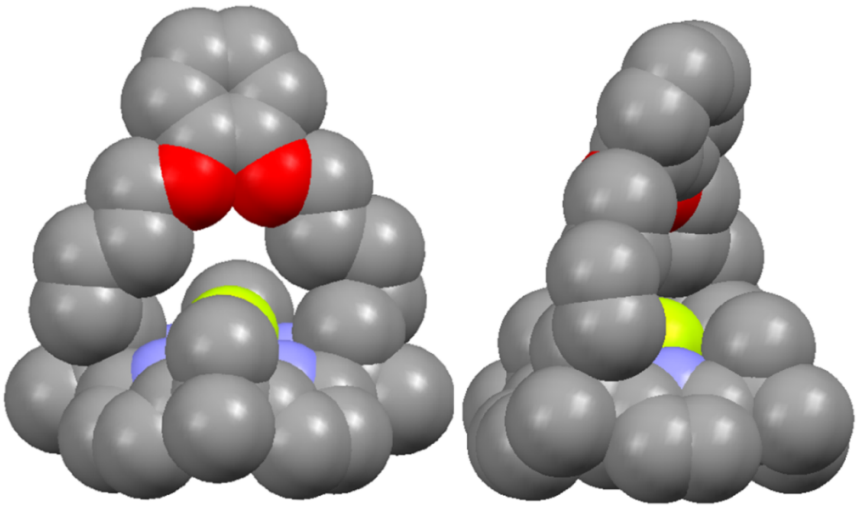


Fig S35: Space-filling model view of DFT optimized structure of **4** with fluoride ion**.** (Hydrogen atoms are removed for clarity.)

In case of **4**-F, the N-H…F, D values ranges from 2.74 Å (169.3°), 2.75 Å (173.3°), 2.74 Å (169.4°), 2.76 Å (174.6°).

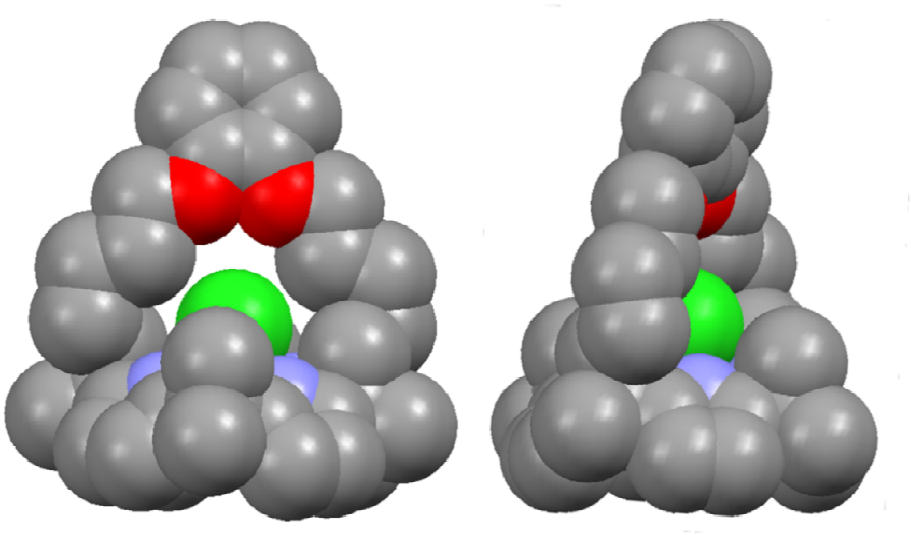


Fig S36: Space-filling model view of DFT optimized structure of **4** with chloride ion**. (**Hydrogen atoms are removed for clarity.)

In case of **4**-Cl, the N-H…Cl, D values ranges from 3.23 Å (173.0°), 3.29 Å (175.2°), 3.31 Å (172.9°), 3.28 Å (174.7°).

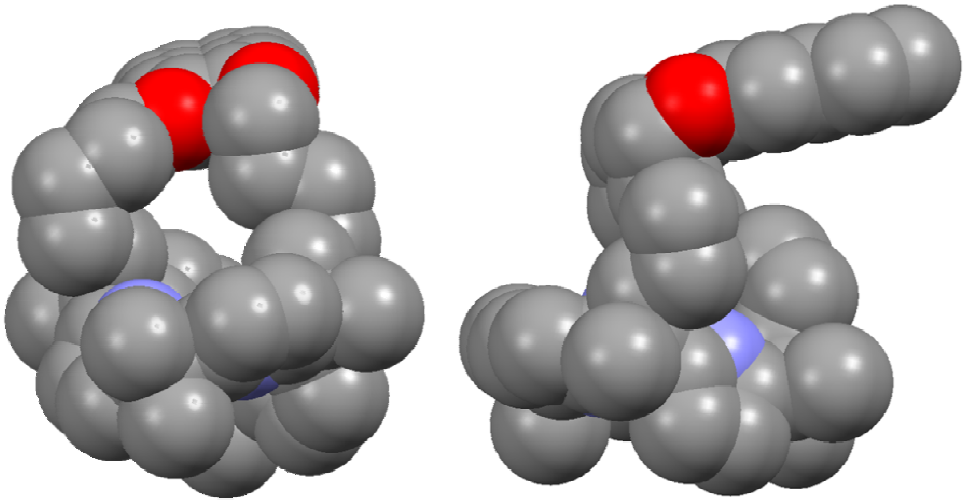


Fig S37: Space-filling model view of DFT optimized structure of **5.** (Hydrogen atoms are removed for clarity.)

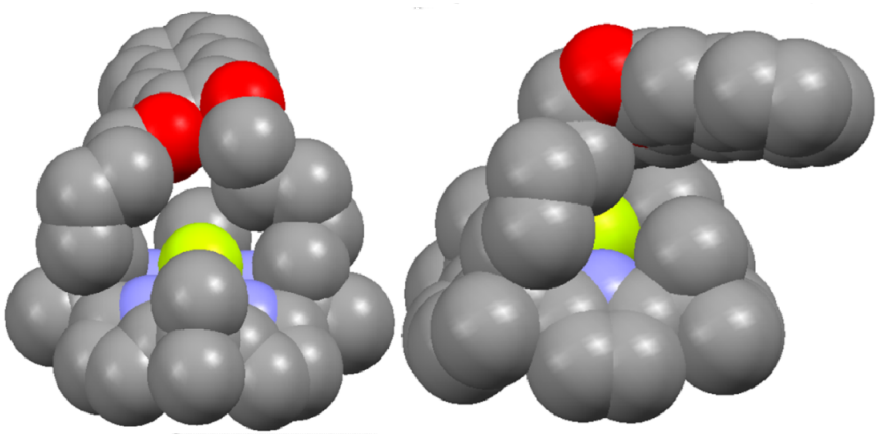


Fig S38: Space-filling model view of DFT optimized structure of **5** with fluoride ion**.** (Hydrogen atoms are removed for clarity.)

In case of **5**-F, the N-H…F, D values ranges from 2.77 Å (174.9°), 2.76 Å (168.4°), 2.77 Å (176.6°), 2.74 Å (169.3°).

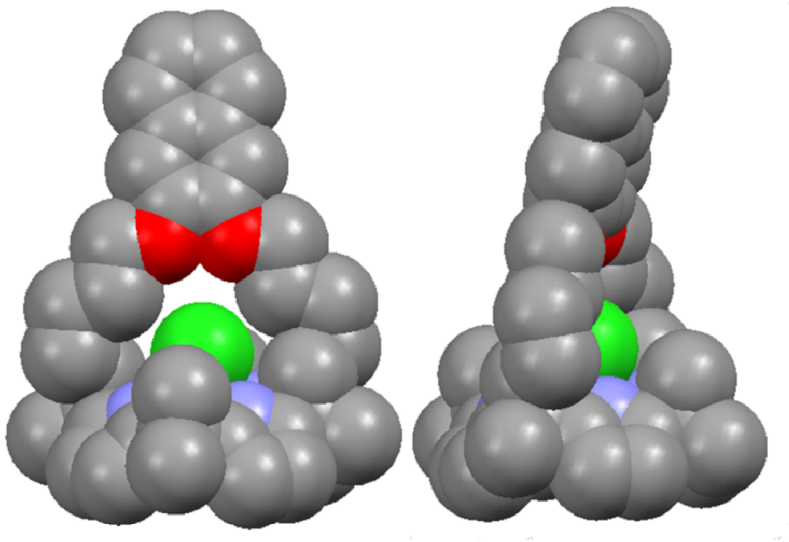


Fig S39: Space-filling model view of DFT optimized structure of **5** with chloride ion**.** (Hydrogen atoms are removed for clarity.)

In case of **5**-Cl, the N-H…Cl, D values ranges from 3.32 Å (172.5°), 3.28 Å (175.7°), 3.28 Å (176.6°), 3.29 Å (174.8°);

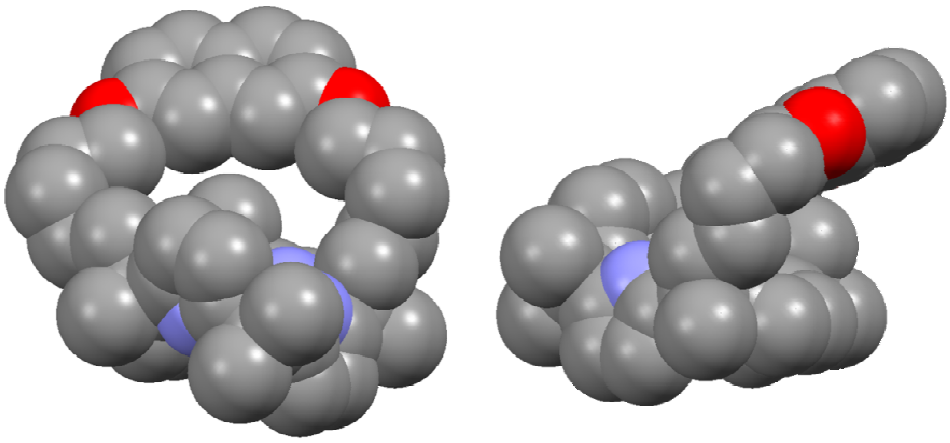


Fig S40: Space-filling model view of DFT optimized structure of **6.** (Hydrogen atoms are removed for clarity.)

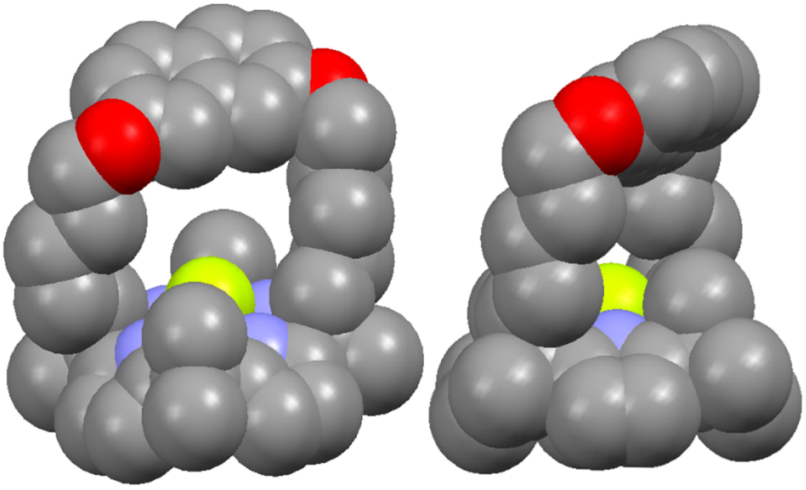


Fig S41: Space-filling model view of DFT optimized structure of **6** with fluoride ion**.** (Hydrogen atoms are removed for clarity.)

In case of **6**-F, the N-H…F, D values ranges from 2.73 Å (173.1°), 2.74 Å (169.4°), 2.74 Å (173.6°), 2.73 Å (169.6°).

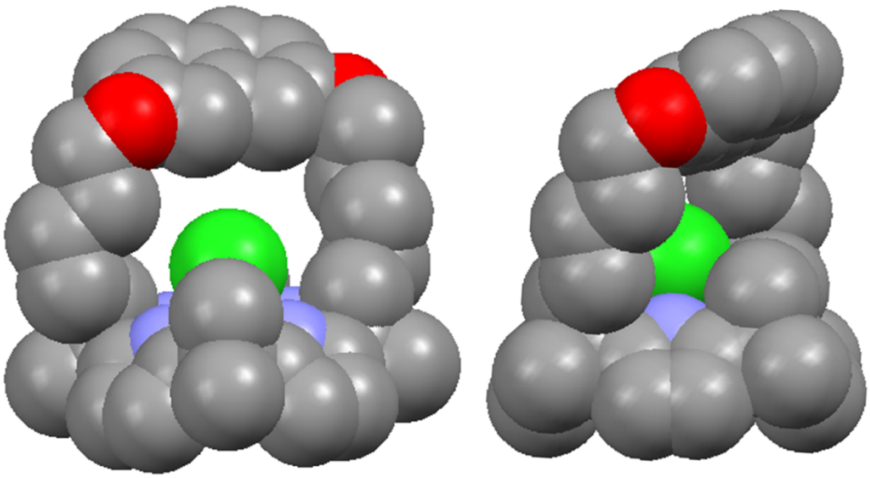


Fig S42: Space-filling model view of DFT optimized structure of **6** with chloride ion**.** (Hydrogen atoms are removed for clarity.)

In case of **6**-Cl, the N-H…Cl, D values ranges from 3.35 Å (173.1°), 3.36 Å (174.0°), 3.36 Å (173.6°), 3.35 Å (176.0°).

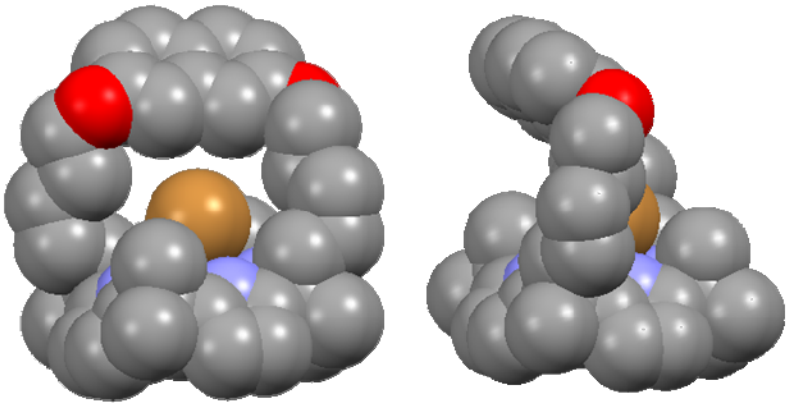


Fig S43: Space-filling model view of DFT optimized structure of **6** with bromide ion**.** (Hydrogen atoms are removed for clarity.)

In case of **6**-Br, the N-H…Br, D values ranges from 3.55 Å (175.6°), 3.53 Å (174.7°), 3.55 Å (175.8°), 3.56 Å (173.8°).

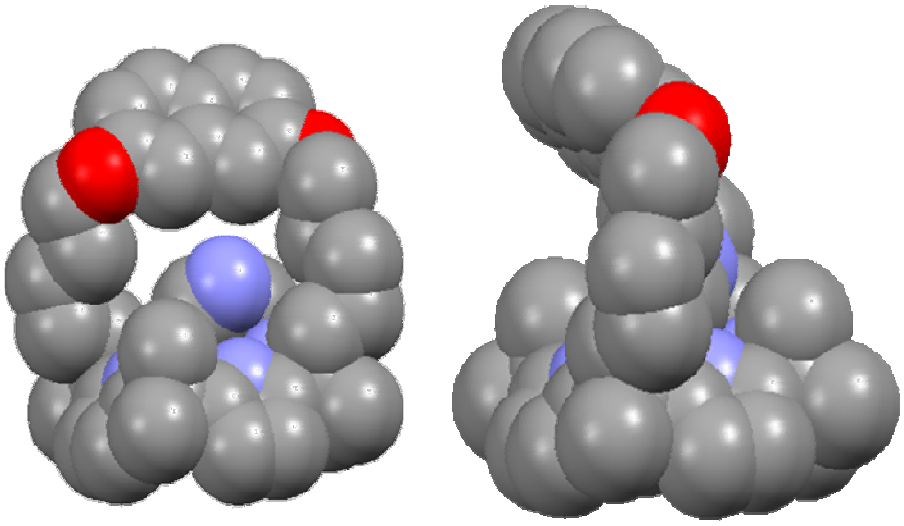


Fig S44: Space-filling model view of DFT optimized structure of **6** with cyanide ion**.** (Hydrogen atoms are removed for clarity.)

In case of **6**-CN, the N-H…CN, D values ranges from 3.38 Å (175.7°), 3.15 Å (161.2°), 3.37 Å (175.5°)3.16 Å (158.4°),.°).(distance measured from anionic oxygen atom)

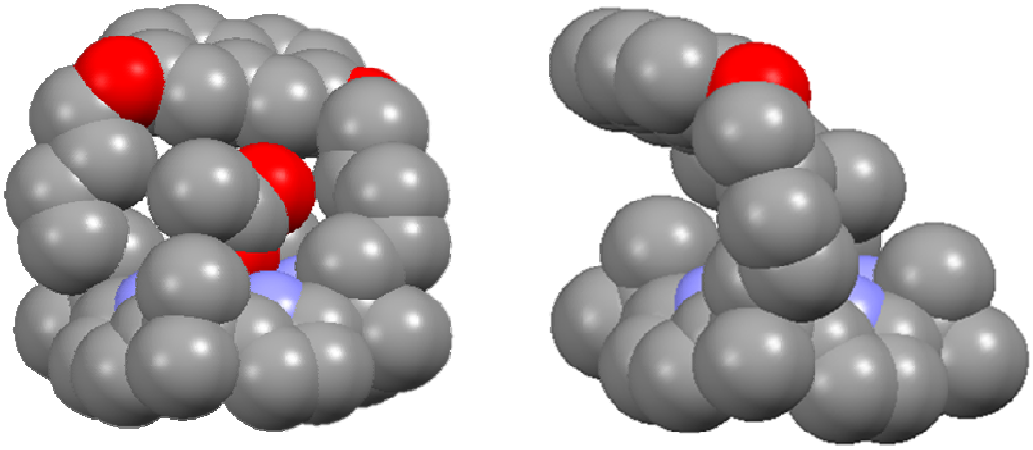


Fig S45: Space-filling model view of DFT optimized structure of **6** with acetate ion**.** (Hydrogen atoms are removed for clarity.)

In case of **6**-OAc, the N-H…OAc, D values ranges from 2.89 Å (170.8°), 2.93 Å (174.4°), 3.09 Å (164.6°), 3.03 Å (168.6°).(distance measured from anionic oxygen atom).

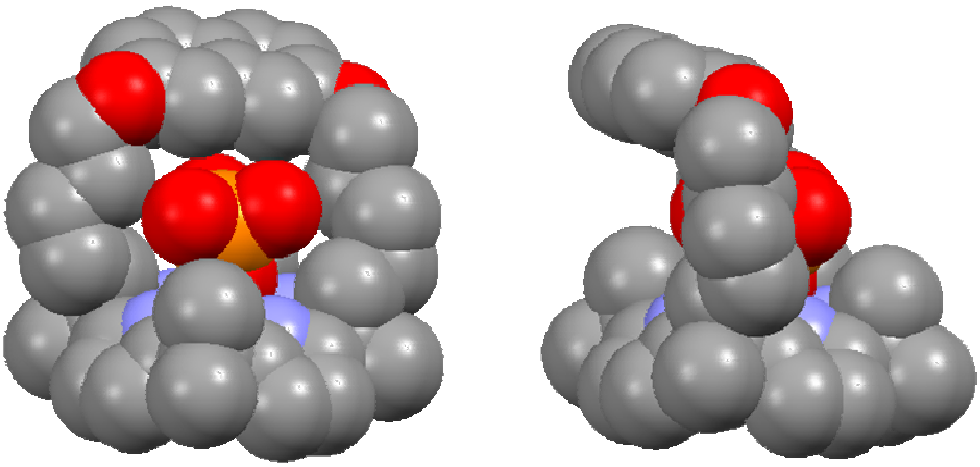


Fig S46: Space-filling model view of DFT optimized structure of **6**with dihydrogenphosphate ion**.** (Hydrogen atoms are removed for clarity.)

In case of **6**-H_2PO_4, the N-H…OH_2PO_4, D values ranges from 2.88 Å (170.9°), 2.97 Å (167.1°), 3.03 Å (167.3°), 3.95 Å (169.4°).(distance measured from anionic oxygen atom).

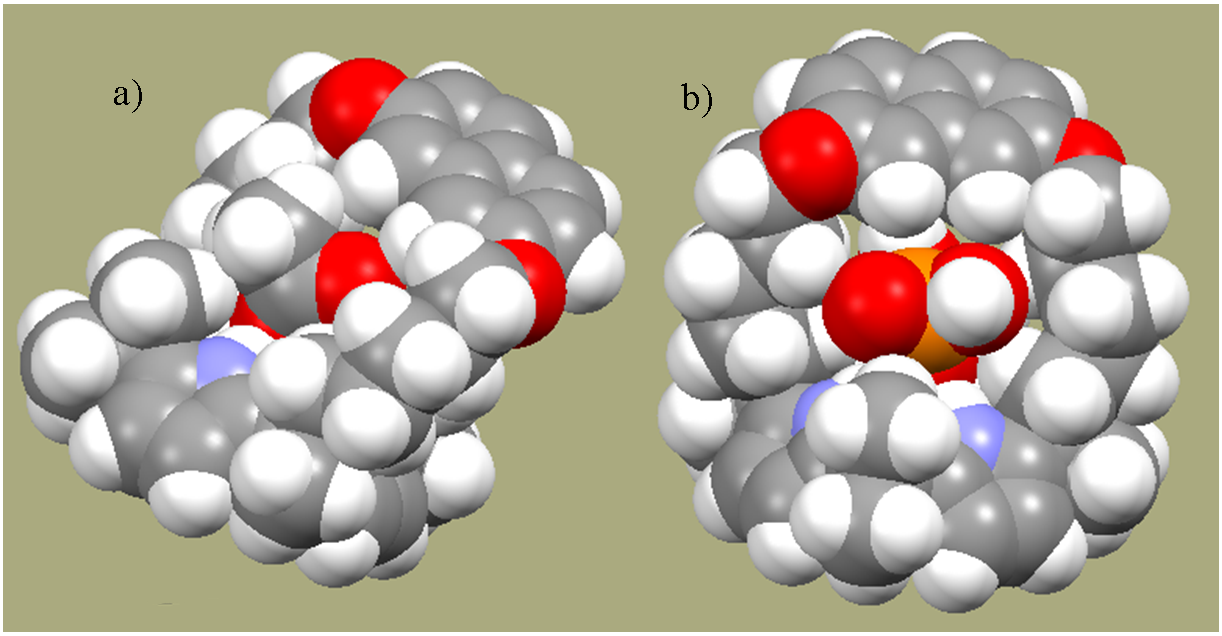


Fig S47: DTF optimized structure of **6** a) with acetate ion and b) with dihydrogenphosphate ion, showing interaction of anion with naphthalene inner C-H atoms.

Cartesian coordinates for the DFT optimized geometry:

Compound **4**

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	1.291087	0.367656	2.599310
2	7	1.999658	2.177896	-0.207884
3	7	2.910830	-0.414493	-1.570102
4	7	1.658168	-2.224708	0.830506
5	6	0.894663	-0.846607	3.127365
6	6	-0.487115	-0.806428	3.205167
7	1	-1.127928	-1.603352	3.562591
8	6	-0.918863	0.459478	2.712680
9	1	-1.943657	0.799732	2.645612
10	6	0.206224	1.173575	2.335259
11	6	0.358756	2.567935	1.723257
12	6	1.720069	2.673573	1.054073
13	6	2.934267	3.064902	1.594795
14	1	3.084685	3.488874	2.580145
15	6	3.953657	2.798628	0.637459
16	1	5.010105	3.003808	0.758722
17	6	3.356857	2.251075	-0.482618
18	6	3.949769	1.897238	-1.837297
19	6	3.377995	0.598585	-2.385011
20	6	3.304061	0.122939	-3.682788
21	1	3.602502	0.660420	-4.575306
22	6	2.779147	-1.201167	-3.636581
23	1	2.564691	-1.833209	-4.490554
24	6	2.536450	-1.516582	-2.310861
25	6	1.746058	-2.661077	-1.679862
26	6	2.208400	-2.890425	-0.249890
27	6	3.283011	-3.610140	0.245300
28	1	3.961158	-4.219112	-0.341194
29	6	3.364623	-3.377667	1.648483
30	1	4.095329	-3.801014	2.328724
31	6	2.337769	-2.518344	1.996065
32	6	1.878764	-1.979228	3.348996
33	6	0.270541	3.627527	2.852050
34	1	-0.698322	3.549625	3.355643
35	1	0.379721	4.642764	2.455858
36	1	1.049243	3.470371	3.604190
37	6	-0.848853	2.757014	0.753108
38	1	-0.957971	1.847421	0.148340
39	1	-1.735215	2.786294	1.397189
40	6	3.652982	3.046986	-2.835830
41	1	4.095225	2.837439	-3.815926
42	1	4.078547	3.984245	-2.462423
43	1	2.575583	3.187160	-2.972454
44	6	5.486841	1.756565	-1.696476

45	1	5.747331	0.965921	-0.985263
46	1	5.940384	2.693224	-1.353452
47	1	5.921336	1.502261	-2.668033
48	6	1.960135	-3.950214	-2.499855
49	1	3.017275	-4.231354	-2.522922
50	1	1.627153	-3.809904	-3.533605
51	1	1.396598	-4.783236	-2.069207
52	6	0.251122	-2.206846	-1.786020
53	1	0.068478	-2.085267	-2.861166
54	1	0.177553	-1.192989	-1.371116
55	6	1.189250	-3.112619	4.145492
56	1	0.333265	-3.518238	3.597042
57	1	0.837049	-2.746986	5.116974
58	1	1.897235	-3.929430	4.316976
59	6	3.105786	-1.489373	4.157216
60	1	3.811358	-2.311422	4.317751
61	1	2.791089	-1.111811	5.136439
62	1	3.649123	-0.691491	3.638869
63	1	2.244127	0.656885	2.422173
64	1	1.314197	1.808989	-0.851157
65	1	0.804185	-1.684270	0.818330
66	1	2.890371	-0.375764	-0.560353
67	6	-0.872502	3.985430	-0.168807
68	1	-0.167641	3.839742	-0.998084
69	1	-0.523484	4.875568	0.369903
70	6	-2.273456	4.295757	-0.743998
71	1	-2.165425	5.112617	-1.467481
72	1	-2.907413	4.694092	0.062006
73	6	-3.011465	3.112905	-1.424476
74	1	-2.294416	2.370327	-1.796686
75	1	-3.568679	3.470613	-2.298591
76	6	-3.995378	2.433556	-0.473288
77	1	-3.502336	2.122088	0.453359
78	1	-4.799999	3.133184	-0.206395
79	6	-0.875764	-3.072571	-1.193462
80	1	-0.656651	-4.139278	-1.326674
81	1	-0.955182	-2.911970	-0.109873
82	6	-2.232181	-2.766342	-1.867300
83	1	-2.198689	-3.148539	-2.898525
84	1	-3.028372	-3.322756	-1.356244
85	6	-2.595739	-1.273872	-1.919857
86	1	-1.789358	-0.714724	-2.410814
87	1	-2.681853	-0.860131	-0.906073
88	6	-3.860510	-0.952762	-2.712789
89	8	-5.088155	-1.376807	-2.082741
90	8	-4.550512	1.273554	-1.110541
91	1	-3.861468	-1.504179	-3.659475
92	1	-3.911269	0.114249	-2.931472
93	6	-5.234076	0.377482	-0.325097
94	6	-5.453371	-0.926352	-0.836863
95	6	-5.728369	0.699088	0.946749
96	6	-6.172742	-1.844389	-0.064865
97	6	-6.445895	-0.232632	1.701389
98	1	-5.571885	1.695435	1.349216
99	6	-6.675180	-1.509456	1.192652

100	1	-6.325452	-2.837347	-0.483751
101	1	-6.823620	0.052038	2.681714
102	1	-7.231897	-2.246890	1.767962

Compound **4**-Fluoride

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	1.845800	-1.269640	-1.980259
2	7	1.757934	-2.029247	1.300303
3	7	1.726274	1.291631	2.058586
4	7	1.751513	2.048157	-1.230505
5	6	2.519992	-0.582667	-2.967973
6	6	3.508812	-1.432462	-3.433426
7	1	4.215727	-1.211661	-4.221686
8	6	3.417696	-2.652153	-2.705153
9	1	4.048133	-3.521381	-2.835792
10	6	2.374648	-2.532632	-1.803671
11	6	1.811186	-3.518089	-0.776817
12	6	2.251862	-3.132895	0.634005
13	6	3.201163	-3.703818	1.463751
14	1	3.788322	-4.585398	1.245134
15	6	3.275919	-2.919309	2.647874
16	1	3.920865	-3.104931	3.495842
17	6	2.370458	-1.879344	2.528573
18	6	1.985961	-0.782863	3.520027
19	6	2.387034	0.619637	3.065745
20	6	3.341281	1.492216	3.560676
21	1	4.030062	1.288402	4.369370
22	6	3.244035	2.709234	2.829397
23	1	3.850956	3.592013	2.978328
24	6	2.231651	2.565647	1.896359
25	6	1.689015	3.537659	0.844957
26	6	2.195703	3.161301	-0.545612
27	6	3.163609	3.753822	-1.337751
28	1	3.720808	4.648526	-1.095787
29	6	3.301755	2.972182	-2.518007
30	1	3.974452	3.172689	-3.340663
31	6	2.415227	1.912787	-2.433939
32	6	2.095056	0.807438	-3.437254
33	6	2.362822	-4.921835	-1.096893
34	1	2.053419	-5.227952	-2.101881
35	1	1.995096	-5.657277	-0.375140
36	1	3.456170	-4.936238	-1.060220
37	6	0.252105	-3.530357	-0.931871
38	1	-0.107422	-2.501630	-0.868980
39	1	0.034640	-3.866000	-1.956633
40	6	0.452327	-0.827660	3.767624
41	1	0.168511	-0.073930	4.511869
42	1	0.163169	-1.817395	4.141248
43	1	-0.121192	-0.632372	2.856429
44	6	2.685747	-1.074591	4.862696
45	1	3.775091	-1.061735	4.757152
46	1	2.390895	-2.060568	5.236460

47	1	2.405605	-0.319693	5.604387
48	6	2.200221	4.952035	1.186963
49	1	3.293556	4.984480	1.204083
50	1	1.836025	5.254831	2.174439
51	1	1.857199	5.679791	0.445752
52	6	0.124619	3.524056	0.924777
53	1	-0.147367	3.814157	1.949997
54	1	-0.220512	2.495310	0.803825
55	6	0.569934	0.808043	-3.735705
56	1	-0.029547	0.600395	-2.843942
57	1	0.332105	0.044176	-4.485654
58	1	0.265447	1.787659	-4.123369
59	6	2.830579	1.118212	-4.756392
60	1	2.521679	2.096284	-5.139241
61	1	2.594563	0.356526	-5.506375
62	1	3.915915	1.134187	-4.615531
63	1	1.076899	-0.886096	-1.433060
64	1	1.037792	-1.408867	0.929899
65	1	1.033459	1.410771	-0.885889
66	1	0.984934	0.889016	1.486547
67	6	-0.563234	-4.366236	0.066988
68	1	-0.357459	-4.009733	1.084179
69	1	-0.253515	-5.419691	0.039434
70	6	-2.088141	-4.296186	-0.188818
71	1	-2.599195	-4.863859	0.603802
72	1	-2.327230	-4.808101	-1.133723
73	6	-2.620918	-2.855961	-0.233409
74	1	-2.252497	-2.343962	-1.126839
75	1	-2.223866	-2.280718	0.609546
76	6	-4.138065	-2.707196	-0.226928
77	1	-4.618237	-3.289646	-1.028858
78	1	-4.574854	-3.025388	0.730921
79	6	-0.647632	4.406938	-0.070222
80	1	-0.400645	5.464765	0.091648
81	1	-0.334184	4.170261	-1.095247
82	6	-2.181371	4.241700	0.046788
83	1	-2.476972	4.397918	1.095898
84	1	-2.671053	5.041208	-0.529576
85	6	-2.690141	2.872401	-0.431250
86	1	-2.157115	2.063099	0.074035
87	1	-2.475672	2.748434	-1.500558
88	6	-4.178463	2.631991	-0.196024
89	8	-4.408981	1.244263	-0.465319
90	8	-4.383197	-1.310826	-0.432048
91	1	-4.809216	3.254025	-0.850018
92	1	-4.458557	2.847850	0.846098
93	6	-5.587304	-0.767729	-0.156634
94	6	-5.597313	0.679608	-0.158372
95	6	-6.743248	-1.459587	0.124724
96	6	-6.757103	1.354104	0.147430
97	6	-7.955792	-0.776705	0.432194
98	1	-6.742141	-2.544969	0.120714
99	6	-7.961672	0.654155	0.448408
100	1	-6.767716	2.439259	0.159614
101	1	-8.848517	-1.325788	0.647719
102	1	-8.857187	1.190724	0.683030
103	9	-0.493663	-0.018327	0.019145

Compound **4**-Chloride

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	17	-0.103099	0.143722	-0.631226
2	7	1.480911	0.951300	2.259378
3	7	2.835167	1.774972	-0.732185
4	7	2.619230	-1.479538	-1.722802
5	7	1.251750	-2.284651	1.256469
6	6	1.516601	0.144351	3.379886
7	6	2.354343	0.765139	4.290297
8	1	2.598032	0.403338	5.281259
9	6	2.827671	1.970889	3.697820
10	1	3.492416	2.688428	4.161897
11	6	2.271186	2.071912	2.433601
12	6	2.401521	3.165562	1.373203
13	6	3.263639	2.696814	0.204386
14	6	4.561173	3.037491	-0.138581
15	1	5.193641	3.741374	0.388416
16	6	4.914044	2.302305	-1.305780
17	1	5.860911	2.351440	-1.829064
18	6	3.825784	1.525405	-1.664196
19	6	3.639422	0.573787	-2.843086
20	6	3.663015	-0.889608	-2.408257
21	6	4.614500	-1.875843	-2.607769
22	1	5.559091	-1.755365	-3.123479
23	6	4.121692	-3.082132	-2.031197
24	1	4.627466	-4.039523	-2.028894
25	6	2.876333	-2.817112	-1.486451
26	6	1.896323	-3.730325	-0.749913
27	6	1.867634	-3.408835	0.741245
28	6	2.381037	-4.109864	1.818952
29	1	2.923918	-5.045646	1.768468
30	6	2.055811	-3.390588	3.004576
31	1	2.308972	-3.680597	4.016710
32	6	1.346998	-2.260607	2.635034
33	6	0.727170	-1.156646	3.485501
34	6	3.088705	4.381444	2.030585
35	1	2.465200	4.775265	2.839880
36	1	3.260715	5.177933	1.302573
37	1	4.059514	4.107102	2.453193
38	6	0.964117	3.571372	0.906766
39	1	0.446740	2.685696	0.523310
40	1	0.413052	3.880766	1.806798
41	6	2.306258	0.888277	-3.573721
42	1	2.195429	0.233434	-4.446071
43	1	2.304881	1.928991	-3.918422
44	1	1.431997	0.745252	-2.931419
45	6	4.788491	0.806080	-3.845485
46	1	5.764601	0.587064	-3.401893
47	1	4.793227	1.848744	-4.178370
48	1	4.660835	0.161311	-4.720816
49	6	2.368868	-5.188693	-0.926325
50	1	3.369399	-5.339897	-0.509966

51	1	2.402739	-5.446457	-1.989650
52	1	1.689026	-5.880716	-0.421548
53	6	0.478134	-3.580602	-1.396115
54	1	0.541165	-3.989195	-2.415072
55	1	0.238208	-2.517891	-1.512343
56	6	-0.747779	-0.923293	3.062084
57	1	-0.844305	-0.594107	2.023012
58	1	-1.203491	-0.157756	3.701181
59	1	-1.318584	-1.852545	3.174224
60	6	0.725367	-1.613413	4.958633
61	1	0.153681	-2.540836	5.064680
62	1	0.265864	-0.846583	5.590477
63	1	1.738994	-1.795470	5.328644
64	1	0.944570	0.745577	1.416904
65	1	1.911344	1.341758	-0.740625
66	1	0.764641	-1.584322	0.696318
67	1	1.770764	-0.990527	-1.436040
68	6	0.870908	4.685799	-0.145849
69	1	1.310654	4.340268	-1.090815
70	1	1.461337	5.554434	0.170084
71	6	-0.571734	5.164206	-0.394853
72	1	-0.539391	6.045923	-1.051948
73	1	-1.003219	5.510152	0.556978
74	6	-1.497876	4.112770	-1.023538
75	1	-1.570113	3.221005	-0.390445
76	1	-1.080215	3.775857	-1.981873
77	6	-2.899587	4.664040	-1.272262
78	1	-3.372675	4.977736	-0.332619
79	1	-2.862353	5.535330	-1.936167
80	6	-0.695783	-4.227324	-0.645394
81	1	-0.508261	-5.291843	-0.454927
82	1	-0.782734	-3.752573	0.338466
83	6	-2.030675	-4.060614	-1.404852
84	1	-1.955862	-3.205098	-2.091291
85	1	-2.220239	-4.940408	-2.036431
86	6	-3.218689	-3.810450	-0.465438
87	1	-3.049161	-2.863715	0.061996
88	1	-3.278154	-4.593819	0.302102
89	6	-4.554621	-3.734628	-1.207164
90	8	-5.598545	-3.168932	-0.394946
91	1	-4.082862	-1.205810	-1.597695
92	6	-4.862685	-0.894264	-0.911754
93	6	-5.044254	0.501151	-0.702907
94	6	-5.659145	-1.809581	-0.249515
95	6	-6.047672	0.955694	0.212503
96	6	-4.251146	1.460822	-1.384964
97	6	-6.661397	-1.359038	0.657168
98	6	-6.844303	-0.016305	0.880028
99	6	-6.213061	2.352289	0.409855
100	6	-4.448570	2.811043	-1.182130
101	1	-3.477168	1.134594	-2.074493
102	1	-7.271260	-2.105592	1.161924
103	1	-7.613028	0.319847	1.575546
104	6	-5.438714	3.266796	-0.270548
105	1	-6.982144	2.697503	1.100655
106	1	-5.597326	4.334764	-0.135881
107	8	-3.733833	3.703555	-1.952630
108	1	-4.917761	-4.734920	-1.463169

109	1	-4.464732	-3.168544	-2.143318

Compound 5

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.102314	-2.432041	1.379536
2	6	-0.223406	-2.303353	1.744206
3	6	-0.313804	-1.252113	2.702554
4	6	0.958837	-0.759361	2.914116
5	7	1.802371	-1.491631	2.102627
6	6	1.808961	-3.426981	0.466888
7	6	1.478388	0.334904	3.827425
8	6	2.203768	1.403608	3.023598
9	6	3.266849	2.222482	3.344666
10	6	3.453297	3.135344	2.266426
11	6	2.501342	2.863794	1.300980
12	7	1.752858	1.805789	1.784297
13	6	2.308866	3.458144	-0.085496
14	6	2.709625	2.441403	-1.147654
15	6	2.326500	2.283654	-2.464598
16	6	3.101443	1.223731	-3.020650
17	6	3.949008	0.754533	-2.036362
18	7	3.695228	1.509090	-0.908759
19	6	4.979152	-0.358822	-2.037700
20	6	4.580244	-1.443862	-1.048556
21	6	5.332706	-2.324991	-0.299923
22	6	4.433217	-3.213185	0.357942
23	6	3.143064	-2.864381	0.002572
24	7	3.258895	-1.784521	-0.853871
25	6	6.370817	0.205757	-1.666107
26	6	5.069245	-0.977205	-3.454269
27	6	0.291655	0.987959	4.577049
28	6	2.440022	-0.271933	4.877487
29	6	2.082844	-4.716648	1.285719
30	6	0.881512	-3.848170	-0.720722
31	6	3.239072	4.692027	-0.226063
32	6	0.854496	3.965626	-0.341009
33	6	0.234704	-2.754110	-1.581442
34	6	-0.277794	2.927643	-0.379588
35	6	-0.837660	-3.297282	-2.547337
36	6	-1.535209	3.423725	-1.111093
37	6	-1.846767	-2.217457	-2.982421
38	6	-2.945269	-2.038003	-1.940026
39	6	-2.531428	2.288031	-1.370739
40	6	-3.801412	2.747412	-2.080840
41	6	-8.534553	0.065472	1.859978
42	6	-8.017851	-1.234416	2.062142
43	6	-6.947382	-1.679890	1.320893
44	6	-6.342382	-0.849560	0.342538
45	6	-6.862598	0.465093	0.142321
46	6	-7.967471	0.895169	0.919896

47	6	-5.243203	-1.288686	-0.443971
48	6	-4.671030	-0.468645	-1.392347
49	6	-5.182627	0.858862	-1.577822
50	6	-6.251383	1.291904	-0.836650
51	8	-4.610108	1.649196	-2.542797
52	8	-3.627607	-0.808853	-2.194820
53	1	-1.044295	-2.899291	1.376440
54	1	-1.215518	-0.904166	3.181072
55	1	2.799375	-1.357087	2.019775
56	1	3.842566	2.189209	4.256020
57	1	4.205400	3.906150	2.213826
58	1	1.016472	1.333938	1.283160
59	1	1.579210	2.863188	-2.983574
60	1	3.041681	0.855246	-4.032599
61	1	4.135225	1.387692	-0.008352
62	1	6.409188	-2.349198	-0.237370
63	1	4.711298	-4.020897	1.015744
64	1	2.493145	-1.252417	-1.236867
65	1	7.127504	-0.582249	-1.693188
66	1	6.659187	0.979976	-2.380629
67	1	6.379361	0.641986	-0.664662
68	1	5.816770	-1.772813	-3.459398
69	1	5.359593	-0.222227	-4.190025
70	1	4.115210	-1.410672	-3.762064
71	1	0.663759	1.773630	5.237500
72	1	-0.240376	0.249451	5.182817
73	1	-0.419224	1.440463	3.882216
74	1	2.792631	0.496054	5.570422
75	1	1.919486	-1.039093	5.454934
76	1	3.314523	-0.729343	4.409399
77	1	2.583788	-5.469777	0.671059
78	1	1.138209	-5.129351	1.643754
79	1	2.706187	-4.508623	2.157237
80	1	0.070955	-4.445716	-0.287390
81	1	1.454251	-4.533468	-1.354991
82	1	4.288090	4.415045	-0.106570
83	1	3.121348	5.127110	-1.220071
84	1	2.993447	5.452628	0.520247
85	1	0.633960	4.730720	0.410732
86	1	0.872989	4.485969	-1.305315
87	1	0.984638	-2.230083	-2.182411
88	1	-0.218149	-2.007411	-0.923754
89	1	0.077119	2.025856	-0.889124
90	1	-0.562364	2.634714	0.636424
91	1	-0.354326	-3.729749	-3.428649
92	1	-1.379287	-4.125088	-2.070899
93	1	-1.241155	3.867767	-2.070451
94	1	-2.009650	4.227469	-0.533815
95	1	-1.334142	-1.261112	-3.126082
96	1	-2.305874	-2.474707	-3.941047
97	1	-2.527315	-2.008401	-0.925711
98	1	-3.649486	-2.877493	-1.992140
99	1	-2.056552	1.522336	-1.991022
100	1	-2.798939	1.805758	-0.423801
101	1	-3.558043	3.301890	-2.989820

102	1	-4.399686	3.401630	-1.433713
103	1	-9.379327	0.406075	2.447958
104	1	-8.469929	-1.882194	2.804959
105	1	-6.553883	-2.679463	1.475872
106	1	-8.362004	1.893715	0.761219
107	1	-4.865114	-2.289012	-0.278975
108	1	-6.637989	2.290506	-1.010691

Compound **5**-Fluoride

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	-0.667452	-1.256761	1.970029
2	7	-3.039451	-1.739507	-0.277264
3	7	-3.294304	1.506765	-0.660122
4	7	-0.837098	1.980213	1.488595
5	6	-0.189470	-0.700467	3.137820
6	6	-0.393224	-1.634452	4.141144
7	1	-0.115065	-1.524025	5.182115
8	6	-1.001251	-2.782003	3.550463
9	1	-1.270990	-3.697500	4.062750
10	6	-1.158580	-2.525009	2.198355
11	6	-1.656160	-3.401708	1.052020
12	6	-2.973260	-2.885374	0.486929
13	6	-4.259348	-3.393580	0.568042
14	1	-4.557409	-4.296297	1.087269
15	6	-5.115705	-2.524912	-0.170012
16	1	-6.180967	-2.651988	-0.319144
17	6	-4.335752	-1.504760	-0.689667
18	6	-4.686012	-0.367066	-1.641960
19	6	-4.531764	1.014898	-1.015356
20	6	-5.441999	2.042943	-0.827281
21	1	-6.505421	1.998521	-1.028433
22	6	-4.720436	3.182196	-0.358466
23	1	-5.138226	4.156695	-0.135781
24	6	-3.384321	2.827177	-0.271058
25	6	-2.131338	3.634693	0.063627
26	6	-1.515752	3.175571	1.379344
27	6	-1.466210	3.784335	2.622163
28	1	-1.893345	4.746021	2.879869
29	6	-0.733669	2.927964	3.495344
30	1	-0.498414	3.124337	4.534175
31	6	-0.348302	1.813306	2.768651
32	6	0.543031	0.636367	3.147250
33	6	-1.864834	-4.832926	1.582710
34	1	-0.922690	-5.234410	1.969885
35	1	-2.226588	-5.495116	0.791263
36	1	-2.599061	-4.851000	2.394295
37	6	-0.536294	-3.406544	-0.046418
38	1	-0.280043	-2.369078	-0.284188
39	1	0.357850	-3.850626	0.414761
40	6	-3.749283	-0.451267	-2.881580
41	1	-4.004236	0.334462	-3.602462
42	1	-3.856507	-1.425814	-3.372444
43	1	-2.699162	-0.324983	-2.599623
44	6	-6.139145	-0.542130	-2.120166

45	1	-6.847152	-0.483154	-1.286879
46	1	-6.263848	-1.515465	-2.605069
47	1	-6.397715	0.239191	-2.841947
48	6	-2.505173	5.124225	0.173785
49	1	-3.239254	5.294913	0.967950
50	1	-2.938957	5.475604	-0.768140
51	1	-1.621742	5.729831	0.397020
52	6	-1.130691	3.427249	-1.123459
53	1	-1.600990	3.848794	-2.023343
54	1	-1.049352	2.354700	-1.307251
55	6	1.726330	0.559934	2.140695
56	1	1.377636	0.373382	1.120378
57	1	2.408800	-0.252092	2.416698
58	1	2.286773	1.502192	2.141083
59	6	1.121198	0.879298	4.553979
60	1	1.679615	1.820361	4.577544
61	1	1.801937	0.067437	4.829016
62	1	0.331368	0.932054	5.310561
63	1	-0.714598	-0.776652	1.059507
64	1	-2.238379	-1.115443	-0.457734
65	1	-0.760020	1.287909	0.730324
66	1	-2.423916	0.956057	-0.644147
67	6	-0.849334	-4.129487	-1.362162
68	1	-1.673159	-3.612042	-1.869788
69	1	-1.199196	-5.151848	-1.168020
70	6	0.358182	-4.213345	-2.318059
71	1	0.029706	-4.721879	-3.233169
72	1	1.124766	-4.867466	-1.875795
73	6	1.003686	-2.858667	-2.705698
74	1	0.284135	-2.038238	-2.589009
75	1	1.300547	-2.875040	-3.761760
76	6	2.247320	-2.538238	-1.881611
77	1	2.008446	-2.436012	-0.816410
78	1	2.997663	-3.334877	-1.988653
79	6	0.291464	3.992953	-0.985799
80	1	0.273190	5.090311	-1.025729
81	1	0.709441	3.722195	-0.008154
82	6	1.211431	3.459920	-2.103887
83	1	0.721896	3.634820	-3.074298
84	1	2.144181	4.040996	-2.126464
85	6	1.552670	1.962434	-1.974126
86	1	0.661011	1.374074	-1.732580
87	1	2.229257	1.817262	-1.121638
88	6	2.198017	1.354709	-3.230265
89	8	3.645598	1.240279	-3.170319
90	8	2.791434	-1.301308	-2.364814
91	1	2.040879	1.998661	-4.101769
92	1	1.777843	0.373292	-3.447114
93	9	-0.958234	0.029489	-0.461972
94	6	3.846084	-0.746784	-1.703506
95	6	4.241393	0.571597	-2.131256
96	6	4.542653	-1.370635	-0.687326
97	6	5.327872	1.175996	-1.538288
98	6	5.666261	-0.754860	-0.070496
99	1	4.255986	-2.363456	-0.351945
100	6	6.077936	0.541967	-0.512704
101	1	5.608347	2.171280	-1.879111
102	6	7.206633	1.153445	0.096415

103	6	6.402579	-1.392672	0.963883
104	6	7.902455	0.509230	1.098414
105	6	7.496560	-0.776165	1.535193
106	1	7.514159	2.142377	-0.243076
107	1	8.766991	0.986870	1.556886
108	1	8.052654	-1.276995	2.326295
109	1	6.088609	-2.381386	1.297862

Compound **5**-Chloride

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	2.620236	-1.277927	-1.907932
2	7	2.337500	-2.031552	1.354387
3	7	2.265759	1.287320	2.114196
4	7	2.502071	2.041410	-1.158547
5	6	3.359853	-0.591795	-2.850171
6	6	4.376988	-1.443835	-3.249301
7	1	5.133739	-1.227731	-3.993504
8	6	4.233803	-2.665718	-2.528124
9	1	4.867590	-3.539128	-2.622478
10	6	3.130831	-2.544779	-1.698839
11	6	2.499393	-3.530041	-0.710999
12	6	2.864334	-3.139603	0.720303
13	6	3.767550	-3.708958	1.602728
14	1	4.363479	-4.595234	1.420556
15	6	3.774218	-2.922288	2.790687
16	1	4.366722	-3.111979	3.677125
17	6	2.874439	-1.883131	2.618915
18	6	2.425531	-0.790849	3.588207
19	6	2.861056	0.610450	3.160244
20	6	3.790552	1.477513	3.711971
21	1	4.426428	1.272866	4.564686
22	6	3.743554	2.697417	2.975573
23	1	4.342727	3.579384	3.166261
24	6	2.784731	2.560931	1.984703
25	6	2.310591	3.538104	0.904357
26	6	2.908765	3.152984	-0.447289
27	6	3.937929	3.732545	-1.170841
28	1	4.485859	4.625098	-0.894117
29	6	4.146289	2.947284	-2.341233
30	1	4.873112	3.144054	-3.119623
31	6	3.240679	1.899284	-2.318141
32	6	2.969807	0.800806	-3.344349
33	6	3.061820	-4.937225	-0.995957
34	1	2.805439	-5.246322	-2.014573
35	1	2.648495	-5.668604	-0.295739
36	1	4.151325	-4.962010	-0.899211
37	6	0.951830	-3.533754	-0.954759
38	1	0.595518	-2.502485	-0.918204
39	1	0.792557	-3.875428	-1.988234
40	6	0.878621	-0.833147	3.731406
41	1	0.546987	-0.083213	4.459319
42	1	0.563678	-1.822417	4.083468

43	1	0.367740	-0.634657	2.784158
44	6	3.033116	-1.086489	4.974434
45	1	4.127278	-1.079018	4.946903
46	1	2.709004	-2.070381	5.327786
47	1	2.706099	-0.332757	5.697454
48	6	2.804039	4.950859	1.277946
49	1	3.893945	4.985129	1.365888
50	1	2.376602	5.256630	2.238482
51	1	2.509116	5.679140	0.517521
52	6	0.744441	3.529048	0.883603
53	1	0.410686	3.822187	1.889667
54	1	0.404421	2.501077	0.741903
55	6	1.464104	0.812103	-3.728000
56	1	0.813312	0.605590	-2.872492
57	1	1.265330	0.054646	-4.495384
58	1	1.188935	1.794151	-4.129991
59	6	3.780903	1.109328	-4.619196
60	1	3.497537	2.087713	-5.019556
61	1	3.584348	0.350594	-5.382970
62	1	4.857314	1.121846	-4.421179
63	1	1.816213	-0.888885	-1.416237
64	1	1.627690	-1.420724	0.947606
65	1	1.745850	1.419796	-0.868633
66	1	1.554420	0.887276	1.501908
67	6	0.076515	-4.363604	-0.002219
68	1	0.222238	-4.002322	1.024302
69	1	0.385189	-5.417373	-0.008216
70	6	-1.430693	-4.290904	-0.345925
71	1	-1.987102	-4.850637	0.420210
72	1	-1.617258	-4.807822	-1.299119
73	6	-1.954220	-2.848941	-0.429094
74	1	-1.536770	-2.347491	-1.307654
75	1	-1.596174	-2.269775	0.428980
76	6	-3.469230	-2.694033	-0.499346
77	1	-3.913020	-3.281469	-1.317181
78	1	-3.952357	-2.999420	0.439264
79	6	0.036819	4.417305	-0.153843
80	1	0.281627	5.472690	0.023283
81	1	0.404659	4.178075	-1.160635
82	6	-1.501994	4.261721	-0.122647
83	1	-1.853857	4.414423	0.909099
84	1	-1.953604	5.066134	-0.720876
85	6	-1.991096	2.898109	-0.636507
86	1	-1.486786	2.083021	-0.111112
87	1	-1.723022	2.785087	-1.695656
88	6	-3.490255	2.662125	-0.476526
89	8	-3.710347	1.272286	-0.769033
90	8	-3.696013	-1.293714	-0.731720
91	1	-4.086724	3.290396	-1.154319
92	1	-3.819020	2.869068	0.552606
93	6	-4.909016	-0.739937	-0.493096
94	6	-4.913369	0.706882	-0.498184
95	6	-6.075226	-1.428842	-0.246103
96	6	-6.078946	1.388837	-0.230838
97	6	-7.293965	-0.738826	0.023959
98	1	-6.083245	-2.515945	-0.248361
99	6	-7.294875	0.692490	0.036449
100	1	-6.090732	2.475778	-0.222837

101	6	-8.508812	1.375601	0.310319
102	6	-8.507690	-1.427915	0.283696
103	6	-9.675030	0.678505	0.559726
104	6	-9.674476	-0.736506	0.545843
105	1	-8.505363	2.465692	0.319666
106	1	-10.598303	1.217235	0.767829
107	1	-10.597369	-1.279886	0.743350
108	1	-8.503258	-2.517991	0.273342
109	17	0.175143	-0.013627	-0.059088

Compound **6**

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.700804	-3.915160	-1.613510
2	6	-0.910710	-5.215325	-1.768248
3	6	0.603726	-4.904375	-1.862618
4	6	1.234032	-4.525282	-0.491272
5	6	-3.659725	3.271224	-0.516098
6	6	-3.721436	4.748632	-0.124754
7	6	-2.467055	5.560492	-0.517598
8	6	-1.140682	5.107876	0.165700
9	6	1.846423	2.931901	-1.147932
10	6	1.658774	2.692245	-2.498751
11	6	2.763086	1.904321	-2.964021
12	6	3.607858	1.678666	-1.890285
13	7	3.034052	2.304057	-0.789753
14	6	1.091912	3.775523	-0.132877
15	6	4.947354	0.977882	-1.774324
16	6	4.877554	-0.059225	-0.671311
17	6	5.708457	-0.353480	0.394610
18	6	5.186835	-1.512187	1.052531
19	6	4.044690	-1.915837	0.382195
20	7	3.860344	-1.008828	-0.662384
21	6	3.080993	-3.059190	0.674115
22	6	2.045922	-2.619967	1.693884
23	6	1.503294	-3.289736	2.775603
24	6	0.494560	-2.455178	3.353271
25	6	0.434562	-1.285954	2.617885
26	7	1.376881	-1.400556	1.597164
27	6	-0.532659	-0.117540	2.700954
28	6	0.166583	1.196547	2.396222
29	6	0.859490	2.061536	3.223880
30	6	1.318534	3.163980	2.435778
31	6	0.902496	2.961840	1.131232
32	7	0.209914	1.752203	1.115842
33	6	-1.677571	-0.368446	1.678125
34	6	-1.144983	-0.047507	4.121168
35	6	6.047957	2.021561	-1.447496
36	6	5.298306	0.284421	-3.117360
37	6	1.952273	5.032326	0.175035
38	6	-0.281682	4.198400	-0.740613
39	6	3.889828	-4.254513	1.235377

40	6	2.365480	-3.488222	-0.653003
41	6	-6.580017	0.988812	-0.115410
42	6	-5.245322	1.396561	-0.393268
43	6	-4.304298	0.460327	-0.765480
44	6	-4.641404	-0.918848	-0.842307
45	6	-5.983499	-1.327711	-0.561306
46	6	-6.935747	-0.332575	-0.204541
47	6	-3.671432	-1.903869	-1.168306
48	6	-4.005544	-3.242031	-1.205357
49	6	-5.344558	-3.645001	-0.946291
50	6	-6.301759	-2.712463	-0.636099
51	8	-5.008073	2.752531	-0.251968
52	8	-3.116305	-4.270406	-1.472104
53	1	-1.370716	-3.359804	-0.726545
54	1	-1.558964	-3.279143	-2.497907
55	1	-1.258464	-5.727857	-2.671534
56	1	-1.119427	-5.863561	-0.910266
57	1	1.132687	-5.767683	-2.281816
58	1	0.743814	-4.076244	-2.573060
59	1	1.608993	-5.432726	-0.005742
60	1	0.476430	-4.098932	0.173995
61	1	-3.412618	3.149738	-1.579380
62	1	-2.919733	2.729861	0.086579
63	1	-3.885377	4.812980	0.956904
64	1	-4.602608	5.175351	-0.617302
65	1	-2.343362	5.533778	-1.609168
66	1	-2.662480	6.606435	-0.252312
67	1	-1.355671	4.595123	1.110888
68	1	-0.556573	6.000325	0.412849
69	1	0.841728	3.051629	-3.101058
70	1	2.919009	1.567477	-3.974850
71	1	3.383200	2.239857	0.160779
72	1	6.597035	0.186842	0.674167
73	1	5.601937	-1.982351	1.927489
74	1	3.131248	-1.045220	-1.362942
75	1	1.785421	-4.270027	3.119953
76	1	-0.116691	-2.701433	4.204428
77	1	1.670305	-0.632907	1.002650
78	1	1.024569	1.925338	4.278935
79	1	1.879420	4.009824	2.795687
80	1	-0.219358	1.354259	0.290876
81	1	-1.272308	-0.515704	0.669596
82	1	-2.389456	0.463438	1.666187
83	1	-2.210121	-1.284837	1.946167
84	1	-0.362128	0.082892	4.873231
85	1	-1.842433	0.792972	4.179059
86	1	-1.688070	-0.972250	4.338974
87	1	5.835444	2.526960	-0.500583
88	1	6.083416	2.769936	-2.244562
89	1	7.024994	1.531999	-1.374448
90	1	4.539599	-0.459054	-3.381786
91	1	5.363019	1.023991	-3.922857
92	1	6.262955	-0.221628	-3.018681
93	1	2.949093	4.733103	0.511220
94	1	2.059411	5.625332	-0.738315

95	1	1.491680	5.647623	0.952800
96	1	-0.843836	3.291767	-0.998631
97	1	-0.081142	4.729547	-1.680072
98	1	3.231363	-5.103287	1.438055
99	1	4.384414	-3.973330	2.168698
100	1	4.647985	-4.556760	0.507177
101	1	1.905155	-2.598411	-1.104802
102	1	3.126213	-3.861126	-1.351542
103	1	-7.288740	1.755991	0.166069
104	1	-3.289332	0.753308	-0.998581
105	1	-7.955267	-0.636667	0.007653
106	1	-2.661654	-1.576037	-1.373977
107	1	-5.568004	-4.702352	-0.993592
108	1	-7.319839	-3.026179	-0.431040

Compound **6**-Fluoride

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	1.791451	0.686784	2.240022
2	7	3.034053	1.401982	-0.653819
3	7	2.404163	-1.658865	-1.643334
4	7	1.077042	-2.337901	1.215881
5	6	1.568440	-0.043425	3.396042
6	6	2.311856	0.547321	4.406397
7	1	2.356669	0.227839	5.434371
8	6	2.994970	1.670923	3.840507
9	1	3.641428	2.350648	4.370193
10	6	2.655310	1.741159	2.496174
11	6	2.933220	2.812701	1.451047
12	6	3.653852	2.279040	0.224586
13	6	4.883192	2.608314	-0.328250
14	1	5.609540	3.282156	0.095034
15	6	5.005912	1.908682	-1.571167
16	1	5.842793	1.957734	-2.247842
17	6	3.847580	1.168490	-1.752746
18	6	3.366393	0.304278	-2.907500
19	6	3.333630	-1.173240	-2.548292
20	6	4.026581	-2.264206	-3.051502
21	1	4.816337	-2.234382	-3.783901
22	6	3.489370	-3.440213	-2.435622
23	1	3.801732	-4.453648	-2.625808
24	6	2.481013	-3.042234	-1.568544
25	6	1.456694	-3.850395	-0.783048

26	6	1.485232	-3.563199	0.707603
27	6	1.724083	-4.395147	1.791681
28	1	2.039355	-5.424366	1.745128
29	6	1.455012	-3.649433	2.983667
30	1	1.538701	-4.013525	3.994174
31	6	1.053283	-2.378545	2.602636
32	6	0.566244	-1.186070	3.408662
33	6	3.779169	3.928453	2.102035
34	1	3.237530	4.351443	2.954069
35	1	3.991063	4.720396	1.379314
36	1	4.729364	3.516898	2.456972
37	6	1.530826	3.374865	1.006968
38	1	0.935105	2.527118	0.649523
39	1	1.035800	3.770807	1.904392
40	6	1.911539	0.743784	-3.274545
41	1	1.551356	0.148564	-4.121355
42	1	1.903757	1.805609	-3.547266
43	1	1.239128	0.589991	-2.424038
44	6	4.285956	0.517168	-4.128214
45	1	5.310104	0.206711	-3.896283
46	1	4.292177	1.576361	-4.404341
47	1	3.920971	-0.076425	-4.972505
48	6	1.711094	-5.354380	-1.021704
49	1	2.704175	-5.631931	-0.654248
50	1	1.657550	-5.570036	-2.093439
51	1	0.962695	-5.953599	-0.495371
52	6	0.043796	-3.451502	-1.348449
53	1	-0.003733	-3.793985	-2.391305
54	1	-0.015087	-2.355940	-1.359365
55	6	-0.765719	-0.672267	2.773765
56	1	-0.597732	-0.338695	1.744738
57	1	-1.150258	0.171065	3.358103
58	1	-1.508568	-1.478487	2.769197
59	6	0.299898	-1.622543	4.864852
60	1	-0.443108	-2.426254	4.878559
61	1	-0.076156	-0.770953	5.440828
62	1	1.221209	-1.985014	5.332653
63	1	1.401168	0.434839	1.312291
64	1	2.133631	0.913673	-0.487106
65	1	0.893685	-1.483521	0.656593
66	1	1.775853	-1.053766	-1.080915
67	6	1.575995	4.461121	-0.087187
68	1	1.974382	4.024845	-1.009866
69	1	2.257691	5.264528	0.216818
70	6	0.186427	5.087588	-0.362017
71	1	0.309645	5.933795	-1.054221
72	1	-0.216301	5.492909	0.577706
73	6	-0.833334	4.098290	-0.970406
74	1	-1.033055	3.277585	-0.273716
75	1	-0.426462	3.662610	-1.890202
76	6	-2.148325	4.807415	-1.307736
77	1	-2.619844	5.201228	-0.398568
78	1	-1.974818	5.630995	-2.006602
79	6	-1.170589	-3.975250	-0.551140
80	1	-1.088108	-5.052650	-0.367685
81	1	-1.176996	-3.477540	0.424072
82	6	-2.498244	-3.674682	-1.294929
83	1	-2.384148	-2.741255	-1.864970

84	1	-2.706884	-4.471579	-2.022398
85	6	-3.690947	-3.497192	-0.329325
86	1	-3.506394	-2.607971	0.283739
87	1	-3.768219	-4.354197	0.349508
88	6	-5.019048	-3.313899	-1.089127
89	8	-6.020139	-2.581754	-0.292700
90	1	-4.191998	-0.894363	-1.486434
91	6	-4.944803	-0.441064	-0.856466
92	6	-4.923210	0.973232	-0.713099
93	6	-5.886616	-1.205040	-0.199318
94	6	-5.881001	1.607236	0.144371
95	6	-3.971050	1.776384	-1.390897
96	6	-6.841368	-0.571379	0.647041
97	6	-6.834303	0.789044	0.814503
98	6	-5.839114	3.019298	0.285629
99	6	-3.967332	3.147411	-1.250393
100	1	-3.233344	1.318904	-2.037695
101	1	-7.559860	-1.206597	1.148117
102	1	-7.561921	1.261530	1.466426
103	6	-4.909802	3.774080	-0.392570
104	1	-6.565404	3.500449	0.933058
105	1	-4.906203	4.853005	-0.300676
106	8	-3.070726	3.892004	-2.017844
107	1	-5.495289	-4.274682	-1.296553
108	1	-4.853021	-2.794965	-2.041494
109	9	0.845299	-0.051751	-0.163348

Compound **6**-Chloride

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	17	-0.083446	0.239125	-0.430805
2	7	1.780343	0.754457	2.282597
3	7	2.902681	1.624826	-0.772392
4	7	2.340899	-1.532283	-1.842802
5	7	1.150295	-2.369875	1.189018
6	6	1.808806	-0.080731	3.393062
7	6	2.717925	0.466036	4.284535
8	1	2.979208	0.064963	5.249167
9	6	3.247498	1.656696	3.698303
10	1	3.976487	2.310840	4.145730
11	6	2.656228	1.821139	2.455346
12	6	2.809905	2.937268	1.427672
13	6	3.516152	2.440342	0.174243
14	6	4.807312	2.671644	-0.272622
15	1	5.552292	3.267807	0.226588
16	6	4.977812	1.977977	-1.509517
17	1	5.873447	1.960786	-2.107008
18	6	3.788192	1.332271	-1.805872
19	6	3.407893	0.476263	-3.006084
20	6	3.342201	-1.001688	-2.646596
21	6	4.147742	-2.060527	-3.035787
22	1	5.016991	-1.996805	-3.668259
23	6	3.618640	-3.253886	-2.453088
24	1	4.020817	-4.246230	-2.568351

25	6	2.497252	-2.908598	-1.715194
26	6	1.525543	-3.773792	-0.920344
27	6	1.651706	-3.513527	0.573611
28	6	2.208510	-4.295131	1.572873
29	1	2.681560	-5.253114	1.438236
30	6	2.043717	-3.608068	2.814663
31	1	2.371827	-3.956439	3.779279
32	6	1.385491	-2.415916	2.560289
33	6	0.933026	-1.319258	3.513277
34	6	3.657508	4.063787	2.065529
35	1	3.143376	4.449483	2.951479
36	1	3.811580	4.875756	1.350624
37	1	4.635645	3.677978	2.367549
38	6	1.380613	3.484795	1.089373
39	1	0.753478	2.652398	0.755351
40	1	0.948628	3.858241	2.027960
41	6	2.031655	0.939106	-3.571167
42	1	1.786519	0.347853	-4.460781
43	1	2.086977	1.998451	-3.847444
44	1	1.227216	0.812055	-2.840316
45	6	4.470875	0.670681	-4.113029
46	1	5.457410	0.348430	-3.766144
47	1	4.521184	1.728295	-4.389385
48	1	4.195609	0.078013	-4.991015
49	6	1.851001	-5.260565	-1.197063
50	1	2.871511	-5.495653	-0.880324
51	1	1.761844	-5.458381	-2.269729
52	1	1.158180	-5.904834	-0.648930
53	6	0.072862	-3.467506	-1.423662
54	1	0.000185	-3.841474	-2.454274
55	1	-0.075411	-2.382529	-1.463421
56	6	-0.551332	-0.944554	3.223925
57	1	-0.681994	-0.546331	2.213322
58	1	-0.880631	-0.182773	3.939463
59	1	-1.181573	-1.834872	3.332266
60	6	1.020493	-1.851641	4.962588
61	1	0.385133	-2.736708	5.065347
62	1	0.679894	-1.077461	5.657154
63	1	2.049825	-2.123552	5.215195
64	1	1.194693	0.606085	1.457898
65	1	1.943229	1.275717	-0.708869
66	1	0.685361	-1.601020	0.699439
67	1	1.592672	-0.985482	-1.410520
68	6	1.335428	4.599383	0.022889
69	1	1.727971	4.211381	-0.924063
70	1	1.979003	5.432659	0.329572
71	6	-0.099934	5.142055	-0.189724
72	1	-0.050219	6.057994	-0.797071
73	1	-0.520507	5.425232	0.786623
74	6	-1.045843	4.138772	-0.887320
75	1	-1.112831	3.200816	-0.326913
76	1	-0.655164	3.891433	-1.881021
77	6	-2.446167	4.733905	-1.054677
78	1	-2.900825	4.944169	-0.078089
79	1	-2.407681	5.659089	-1.639370
80	6	-1.073641	-4.046297	-0.565122
81	1	-0.939685	-5.120849	-0.393190
82	1	-1.052936	-3.552752	0.411818

83	6	-2.443307	-3.786843	-1.243202
84	1	-2.383800	-2.842570	-1.802898
85	1	-2.655718	-4.581751	-1.971959
86	6	-3.602626	-3.658499	-0.230812
87	1	-3.416998	-2.779576	0.396082
88	1	-3.642511	-4.533103	0.428716
89	6	-4.952051	-3.485432	-0.953733
90	8	-5.960187	-2.808514	-0.121610
91	1	-4.111112	-1.040517	-1.170816
92	6	-4.953660	-0.620725	-0.639045
93	6	-5.037206	0.796398	-0.551242
94	6	-5.910170	-1.423178	-0.052823
95	6	-6.120529	1.392280	0.174485
96	6	-4.075001	1.637397	-1.168807
97	6	-6.978211	-0.828456	0.677999
98	6	-7.075913	0.534217	0.789409
99	6	-6.198996	2.808294	0.242735
100	6	-4.198914	3.008555	-1.114897
101	1	-3.223823	1.207301	-1.681407
102	1	-7.702127	-1.493834	1.130026
103	1	-7.895326	0.978224	1.345696
104	6	-5.268084	3.599120	-0.389890
105	1	-7.019924	3.260094	0.790809
106	1	-5.351793	4.678773	-0.366242
107	8	-3.298764	3.801255	-1.829759
108	1	-5.401656	-4.453375	-1.188088
109	1	-4.817247	-2.926629	-1.888724

Compound **6**-Bromide

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	1.316735	1.035498	2.351104
2	7	2.237381	2.282664	-0.685927
3	7	2.689812	-0.904942	-1.860080
4	7	1.778147	-2.158976	1.185047
5	6	1.629440	0.201154	3.406408
6	6	2.406264	0.937249	4.278069
7	1	2.822996	0.586150	5.208729
8	6	2.562797	2.240513	3.730140
9	1	3.117735	3.050198	4.175789
10	6	1.880196	2.284160	2.529477
11	6	1.716482	3.435691	1.538246
12	6	2.553928	3.215107	0.282442
13	6	3.707531	3.846949	-0.137916
14	1	4.227562	4.632441	0.386954
15	6	4.090479	3.277270	-1.384462
16	1	4.953057	3.552980	-1.969919
17	6	3.164896	2.305728	-1.709408
18	6	3.090181	1.384475	-2.922559
19	6	3.502475	-0.039313	-2.564733
20	6	4.673868	-0.720627	-2.828917
21	1	5.527176	-0.333424	-3.362828
22	6	4.558693	-2.022374	-2.266583
23	1	5.309422	-2.795455	-2.303603

24	6	3.318082	-2.119215	-1.665545
25	6	2.676985	-3.290905	-0.923448
26	6	2.645831	-3.048445	0.582340
27	6	3.397788	-3.614497	1.592851
28	1	4.172522	-4.354477	1.468783
29	6	2.971896	-3.047115	2.826731
30	1	3.367841	-3.279279	3.802688
31	6	1.964663	-2.142857	2.553029
32	6	1.161574	-1.247941	3.490895
33	6	2.211442	4.721922	2.234013
34	1	1.593995	4.934931	3.110006
35	1	2.167553	5.574914	1.556849
36	1	3.245642	4.616942	2.565099
37	6	0.201000	3.596900	1.182284
38	1	-0.168801	2.663139	0.750239
39	1	-0.340881	3.729452	2.127117
40	6	1.661962	1.400052	-3.525960
41	1	1.627092	0.762295	-4.414313
42	1	1.394173	2.419973	-3.817744
43	1	0.902261	1.042198	-2.829021
44	6	4.052746	1.917221	-4.003996
45	1	5.087151	1.934891	-3.656051
46	1	3.771334	2.934771	-4.284722
47	1	4.003580	1.282434	-4.891683
48	6	3.532848	-4.545392	-1.198798
49	1	4.568376	-4.389429	-0.892857
50	1	3.525291	-4.777398	-2.266749
51	1	3.151237	-5.405980	-0.649011
52	6	1.232581	-3.523901	-1.475372
53	1	1.305902	-3.594295	-2.567421
54	1	0.620619	-2.640712	-1.272664
55	6	-0.351860	-1.347802	3.171720
56	1	-0.595014	-1.017126	2.160937
57	1	-0.920958	-0.728102	3.870787
58	1	-0.685313	-2.384758	3.273057
59	6	1.362572	-1.746310	4.936802
60	1	1.022543	-2.780834	5.024568
61	1	0.785198	-1.127870	5.627822
62	1	2.410359	-1.706305	5.240083
63	1	0.743988	0.763853	1.556230
64	1	1.429644	1.665217	-0.655762
65	1	1.099564	-1.585735	0.689147
66	1	1.753013	-0.676317	-1.535986
67	6	-0.139645	4.756017	0.234626
68	1	0.349058	4.597395	-0.732877
69	1	0.268651	5.690149	0.632618
70	6	-1.648387	4.964499	0.017984
71	1	-1.788563	5.909218	-0.524846
72	1	-2.135688	5.100820	0.993166
73	6	-2.356749	3.843835	-0.754653
74	1	-2.316200	2.903318	-0.198983
75	1	-1.842351	3.664671	-1.704916
76	6	-3.810202	4.202963	-1.047348
77	1	-4.360314	4.387183	-0.115342
78	1	-3.864740	5.111002	-1.654485

79	6	0.514917	-4.772397	-0.940836
80	1	1.037273	-5.666251	-1.295664
81	1	0.575123	-4.796849	0.153191
82	6	-0.958711	-4.875424	-1.375873
83	1	-1.047665	-4.565385	-2.425961
84	1	-1.261836	-5.930183	-1.347178
85	6	-1.945888	-4.074570	-0.512465
86	1	-1.670121	-3.017022	-0.481530
87	1	-1.906474	-4.444655	0.517897
88	6	-3.374299	-4.249942	-1.026760
89	8	-4.389962	-3.885347	-0.079996
90	1	-3.401367	-1.601931	-1.246502
91	6	-4.320059	-1.522295	-0.681179
92	6	-4.931786	-0.243435	-0.575649
93	6	-4.869041	-2.608342	-0.035695
94	6	-6.109614	-0.085101	0.218430
95	6	-4.388265	0.891133	-1.232160
96	6	-6.036640	-2.452417	0.760335
97	6	-6.634306	-1.226367	0.881629
98	6	-6.704444	1.197971	0.314956
99	6	-4.992433	2.120537	-1.118041
100	1	-3.479769	0.794250	-1.814234
101	1	-6.433280	-3.328986	1.259026
102	1	-7.526294	-1.116580	1.490880
103	6	-6.165399	2.280312	-0.338566
104	1	-7.605454	1.314467	0.909804
105	1	-6.632308	3.257236	-0.282132
106	8	-4.493200	3.198584	-1.820694
107	1	-3.564632	-5.309981	-1.218031
108	1	-3.533863	-3.707853	-1.965557
109	35	-0.462360	-0.023627	-0.542780

Compound **6** – cyanide

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	1.357253	1.059064	2.299833
2	7	2.242601	2.222428	-0.708622
3	7	2.526696	-1.036504	-1.909656
4	7	1.635260	-2.211840	1.149793
5	6	1.590820	0.213198	3.366711
6	6	2.367839	0.916650	4.271343
7	1	2.732124	0.547493	5.219452
8	6	2.604421	2.212420	3.729055
9	1	3.175461	3.001545	4.196479
10	6	1.968697	2.281894	2.499960
11	6	1.863788	3.438372	1.505862
12	6	2.642015	3.161946	0.222215
13	6	3.789494	3.755069	-0.276701
14	1	4.359428	4.539162	0.201314
15	6	4.081961	3.151989	-1.534142
16	1	4.916583	3.392240	-2.177290
17	6	3.108314	2.199772	-1.785284

18	6	2.936558	1.255352	-2.973534
19	6	3.343132	-0.171850	-2.614692
20	6	4.522240	-0.853155	-2.861010
21	1	5.382540	-0.463997	-3.386602
22	6	4.406325	-2.151644	-2.287816
23	1	5.162627	-2.922986	-2.306928
24	6	3.157337	-2.248585	-1.697093
25	6	2.515152	-3.407396	-0.933806
26	6	2.488506	-3.131257	0.567858
27	6	3.242720	-3.673861	1.593711
28	1	4.011311	-4.425917	1.486502
29	6	2.831796	-3.061513	2.812842
30	1	3.233896	-3.265094	3.795029
31	6	1.830395	-2.152807	2.517231
32	6	1.048021	-1.212662	3.431396
33	6	2.459496	4.694100	2.178135
34	1	1.884672	4.949442	3.073982
35	1	2.443127	5.547416	1.496767
36	1	3.497954	4.525855	2.475927
37	6	0.348945	3.691094	1.189760
38	1	-0.082616	2.771812	0.781862
39	1	-0.158694	3.868841	2.148310
40	6	1.473410	1.293417	-3.488053
41	1	1.368273	0.642259	-4.363167
42	1	1.211283	2.316451	-3.779475
43	1	0.746982	0.965017	-2.741528
44	6	3.840540	1.746487	-4.125530
45	1	4.896497	1.751864	-3.842462
46	1	3.561382	2.765225	-4.411724
47	1	3.725485	1.092080	-4.994935
48	6	3.370511	-4.668943	-1.183753
49	1	4.408528	-4.510904	-0.880144
50	1	3.362262	-4.922366	-2.248712
51	1	2.985354	-5.519486	-0.616980
52	6	1.069961	-3.651799	-1.481387
53	1	1.145457	-3.752814	-2.572807
54	1	0.455487	-2.763408	-1.305855
55	6	-0.460537	-1.232497	3.068140
56	1	-0.662021	-0.883414	2.052990
57	1	-1.015561	-0.585489	3.756099
58	1	-0.852359	-2.252077	3.152970
59	6	1.177406	-1.723227	4.883203
60	1	0.782427	-2.740999	4.957292
61	1	0.610678	-1.075607	5.559118
62	1	2.217354	-1.737591	5.220899
63	1	0.818201	0.812245	1.467702
64	1	1.428088	1.615088	-0.599600
65	1	0.954314	-1.656714	0.642963
66	1	1.583200	-0.815729	-1.609032
67	6	0.049707	4.853552	0.231304
68	1	0.555894	4.680067	-0.726869
69	1	0.466516	5.784436	0.634654
70	6	-1.452427	5.080793	-0.021540
71	1	-1.567648	6.015988	-0.589933
72	1	-1.961870	5.244376	0.940162

73	6	-2.155260	3.948728	-0.786592
74	1	-2.156206	3.024951	-0.198353
75	1	-1.607804	3.729539	-1.712019
76	6	-3.591823	4.318332	-1.148418
77	1	-4.174528	4.547463	-0.244476
78	1	-3.609705	5.203108	-1.794497
79	6	0.345547	-4.884124	-0.914431
80	1	0.845278	-5.793848	-1.268649
81	1	0.427801	-4.894226	0.180515
82	6	-1.140436	-4.960558	-1.315327
83	1	-1.242147	-4.683941	-2.375762
84	1	-1.476693	-6.005134	-1.240761
85	6	-2.078374	-4.090998	-0.460526
86	1	-1.748985	-3.047190	-0.463740
87	1	-2.046153	-4.439982	0.579735
88	6	-3.520451	-4.202339	-0.956689
89	8	-4.503661	-3.762118	-0.006064
90	1	-3.363695	-1.537163	-1.172248
91	6	-4.301003	-1.410532	-0.642815
92	6	-4.860849	-0.102455	-0.577459
93	6	-4.922425	-2.460926	0.005241
94	6	-6.055287	0.124382	0.181044
95	6	-4.252173	0.994722	-1.247494
96	6	-6.104041	-2.237866	0.768463
97	6	-6.649097	-0.980099	0.853340
98	6	-6.599720	1.435090	0.231439
99	6	-4.812622	2.252565	-1.182052
100	1	-3.334748	0.842431	-1.806718
101	1	-6.555322	-3.087859	1.270744
102	1	-7.552670	-0.818044	1.436806
103	6	-6.000069	2.480728	-0.436802
104	1	-7.511998	1.602577	0.799960
105	1	-6.430808	3.477510	-0.418163
106	8	-4.255987	3.289960	-1.906797
107	1	-3.772181	-5.255962	-1.124287
108	1	-3.660711	-3.667126	-1.904826
109	7	-0.735155	-0.647720	-0.885737
110	6	-0.171914	0.228421	-0.336321

Compound **6**- acetate

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	0.858427	1.060118	2.192371
2	7	2.672984	2.214640	-0.400890
3	7	3.293542	-0.972809	-1.305154
4	7	1.434229	-2.112795	1.249567
5	6	0.757294	0.266263	3.316318
6	6	1.180893	1.030109	4.385043
7	1	1.220804	0.713752	5.415265
8	6	1.542856	2.313938	3.887375
9	1	1.901627	3.142928	4.476205
10	6	1.335621	2.313474	2.521932

11	6	1.468612	3.440836	1.500361
12	6	2.645347	3.207986	0.558813
13	6	3.870330	3.844827	0.511637
14	1	4.183529	4.668142	1.133622
15	6	4.653283	3.211925	-0.492524
16	1	5.659625	3.478690	-0.773220
17	6	3.895445	2.197746	-1.045560
18	6	4.234995	1.243166	-2.186818
19	6	4.361003	-0.212419	-1.745736
20	6	5.458973	-1.048968	-1.777726
21	1	6.456325	-0.777253	-2.084887
22	6	5.040684	-2.336532	-1.342646
23	1	5.669389	-3.207792	-1.255468
24	6	3.691466	-2.270927	-1.049744
25	6	2.758947	-3.363650	-0.527290
26	6	2.342634	-3.095377	0.912814
27	6	2.694893	-3.733618	2.085465
28	1	3.381980	-4.560153	2.176001
29	6	1.979845	-3.115306	3.150276
30	1	2.028728	-3.388034	4.192658
31	6	1.201521	-2.111083	2.609086
32	6	0.216848	-1.156323	3.268582
33	6	1.714145	4.751571	2.276964
34	1	0.860541	4.969000	2.923276
35	1	1.861752	5.590498	1.596001
36	1	2.603357	4.675223	2.904453
37	6	0.098577	3.544720	0.750885
38	1	-0.115602	2.586648	0.273365
39	1	-0.662883	3.664965	1.531313
40	6	3.159314	1.349438	-3.298462
41	1	3.429028	0.708954	-4.143510
42	1	3.077159	2.382874	-3.648696
43	1	2.181166	1.036243	-2.939828
44	6	5.577364	1.683266	-2.805626
45	1	6.392665	1.629824	-2.081586
46	1	5.503563	2.712556	-3.163643
47	1	5.828554	1.039824	-3.651639
48	6	3.534321	-4.697570	-0.575750
49	1	4.457528	-4.636666	0.002584
50	1	3.795382	-4.944399	-1.608060
51	1	2.936762	-5.510059	-0.163178
52	6	1.480190	-3.479740	-1.427187
53	1	1.805313	-3.516916	-2.473756
54	1	0.878208	-2.573430	-1.326750
55	6	-1.135110	-1.182735	2.507297
56	1	-1.041165	-0.885021	1.461670
57	1	-1.847090	-0.504962	2.986688
58	1	-1.550887	-2.193993	2.521591
59	6	-0.048035	-1.634316	4.709544
60	1	-0.452708	-2.648782	4.696071
61	1	-0.772580	-0.976387	5.194819
62	1	0.864404	-1.638972	5.309271
63	1	0.659832	0.745583	1.245725
64	1	1.913158	1.551942	-0.574859
65	1	1.021328	-1.455561	0.590475

66	1	2.354825	-0.611219	-1.141749
67	6	-0.070406	4.667763	-0.284658
68	1	0.418829	4.389814	-1.224750
69	1	0.429986	5.578279	0.056747
70	6	-1.549036	5.016846	-0.543802
71	1	-1.597924	5.882112	-1.217826
72	1	-1.997435	5.343768	0.404402
73	6	-2.390275	3.877619	-1.135959
74	1	-2.317731	2.984598	-0.509359
75	1	-2.000743	3.606065	-2.122537
76	6	-3.860743	4.259263	-1.286196
77	1	-4.312748	4.457170	-0.305646
78	1	-3.961366	5.163825	-1.892634
79	6	0.599340	-4.707302	-1.124268
80	1	1.096348	-5.600298	-1.516032
81	1	0.533621	-4.847814	-0.039570
82	6	-0.830080	-4.647918	-1.706757
83	1	-0.823632	-4.080563	-2.645939
84	1	-1.143504	-5.667250	-1.969543
85	6	-1.875480	-4.051868	-0.749320
86	1	-1.631161	-3.011435	-0.527571
87	1	-1.860615	-4.611981	0.192732
88	6	-3.281595	-4.152920	-1.335866
89	8	-4.322627	-3.847508	-0.388841
90	1	-3.401931	-1.509504	-1.508176
91	6	-4.308919	-1.468603	-0.920183
92	6	-4.935322	-0.205018	-0.750167
93	6	-4.814707	-2.580217	-0.282522
94	6	-6.071452	-0.077776	0.107226
95	6	-4.449762	0.950401	-1.416756
96	6	-5.947733	-2.460689	0.569801
97	6	-6.551069	-1.245365	0.760076
98	6	-6.669156	1.198013	0.267013
99	6	-5.058387	2.170998	-1.247862
100	1	-3.593759	0.864115	-2.073255
101	1	-6.311754	-3.355517	1.061282
102	1	-7.412111	-1.165533	1.416740
103	6	-6.180196	2.302392	-0.391977
104	1	-7.536078	1.292868	0.914236
105	1	-6.654343	3.271872	-0.287129
106	8	-4.629016	3.261681	-1.983131
107	1	-3.489163	-5.186484	-1.629559
108	1	-3.392059	-3.523913	-2.224747
109	6	-0.344846	-0.012931	-1.481236
110	8	0.662198	0.164604	-0.692591
111	6	-0.464190	0.930311	-2.682246
112	1	-1.510960	1.072853	-2.950453
113	1	0.009860	1.895328	-2.501425
114	1	0.032090	0.462623	-3.538364
115	8	-1.187938	-0.908695	-1.355822

Compound **6**- dihydrogenphosphate

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	-1.256178	-1.117297	2.308807
2	7	-2.606474	-2.165648	-0.579094
3	7	-3.075843	1.060807	-1.511248
4	7	-1.703648	2.112188	1.377003
5	6	-1.370960	-0.355480	3.455760
6	6	-1.959241	-1.163458	4.413429
7	1	-2.188330	-0.880056	5.430742
8	6	-2.200255	-2.437064	3.822586
9	1	-2.644742	-3.290466	4.313817
10	6	-1.756189	-2.390186	2.511504
11	6	-1.726157	-3.480799	1.439125
12	6	-2.733044	-3.202673	0.324496
13	6	-3.913854	-3.857507	0.013988
14	1	-4.317299	-4.718105	0.528101
15	6	-4.504276	-3.192694	-1.098557
16	1	-5.431614	-3.464268	-1.582300
17	6	-3.676243	-2.140461	-1.453663
18	6	-3.792257	-1.144610	-2.606729
19	6	-4.034336	0.292832	-2.145602
20	6	-5.144942	1.103348	-2.313574
21	1	-6.075038	0.818928	-2.784330
22	6	-4.842755	2.381035	-1.762208
23	1	-5.506746	3.232853	-1.737654
24	6	-3.550746	2.335209	-1.263410
25	6	-2.729579	3.421079	-0.562216
26	6	-2.540144	3.112955	0.920373
27	6	-3.085943	3.718124	2.039375
28	1	-3.780647	4.545970	2.038916
29	6	-2.565397	3.059274	3.190651
30	1	-2.794845	3.297775	4.219347
31	6	-1.708739	2.061346	2.758112
32	6	-0.857207	1.077941	3.555117
33	6	-2.112717	-4.813441	2.118548
34	1	-1.385544	-5.061353	2.897839
35	1	-2.139193	-5.629758	1.393503
36	1	-3.100611	-4.748791	2.581770
37	6	-0.254828	-3.599427	0.903578
38	1	0.078653	-2.623323	0.542098
39	1	0.372342	-3.823660	1.778139
40	6	-2.513154	-1.211099	-3.486740
41	1	-2.597404	-0.502578	-4.319096
42	1	-2.394486	-2.221020	-3.894807
43	1	-1.600763	-0.984978	-2.932495
44	6	-4.980140	-1.571112	-3.496283
45	1	-5.926776	-1.549757	-2.948625
46	1	-4.822065	-2.587879	-3.867542
47	1	-5.064949	-0.897378	-4.354198
48	6	-3.509542	4.748776	-0.688234
49	1	-4.513843	4.657019	-0.266892

50	1	-3.606323	5.030051	-1.741902
51	1	-3.000100	5.554884	-0.156107
52	6	-1.338713	3.572293	-1.271167
53	1	-1.531624	3.704802	-2.344942
54	1	-0.777140	2.638686	-1.181058
55	6	0.618729	1.143623	3.075197
56	1	0.746082	0.840538	2.034189
57	1	1.237692	0.476510	3.685622
58	1	0.998317	2.166540	3.176962
59	6	-0.878795	1.503093	5.038829
60	1	-0.488556	2.520041	5.142377
61	1	-0.252759	0.827693	5.629611
62	1	-1.890405	1.481757	5.454379
63	1	-0.899236	-0.770265	1.421414
64	1	-1.843264	-1.490863	-0.586073
65	1	-1.199756	1.463185	0.774564
66	1	-2.160483	0.717414	-1.218307
67	6	0.004563	-4.643087	-0.196454
68	1	-0.388281	-4.272257	-1.150178
69	1	-0.540887	-5.568137	0.024464
70	6	1.494367	-5.012109	-0.368480
71	1	1.562560	-5.809313	-1.123922
72	1	1.866777	-5.448536	0.571541
73	6	2.398794	-3.844553	-0.797031
74	1	2.431359	-3.091883	-0.000971
75	1	1.970139	-3.343103	-1.670378
76	6	3.820265	-4.292869	-1.128355
77	1	4.353477	-4.643551	-0.232854
78	1	3.809803	-5.111165	-1.855270
79	6	-0.463984	4.737531	-0.773090
80	1	-0.971426	5.683122	-0.995202
81	1	-0.374252	4.690166	0.319680
82	6	0.948921	4.789020	-1.406102
83	1	0.912607	4.350479	-2.413634
84	1	1.238075	5.841162	-1.543715
85	6	2.050687	4.098164	-0.582633
86	1	1.809214	3.042773	-0.433284
87	1	2.111832	4.569271	0.406714
88	6	3.417884	4.236135	-1.256604
89	8	4.515486	3.908615	-0.384225
90	1	3.782520	1.633620	-1.749750
91	6	4.533267	1.534246	-0.975209
92	6	5.032508	0.231888	-0.681521
93	6	4.937567	2.620887	-0.222985
94	6	5.951250	0.053100	0.403703
95	6	4.589607	-0.918399	-1.396867
96	6	5.888836	2.451036	0.824698
97	6	6.375288	1.203371	1.126447
98	6	6.379223	-1.259939	0.731457
99	6	5.008199	-2.187233	-1.034757
100	1	3.905418	-0.818593	-2.235181
101	1	6.191537	3.329596	1.385382
102	1	7.081265	1.079985	1.944334
103	6	5.918150	-2.361356	0.041722
104	1	7.081720	-1.390194	1.551650

105	1	6.257419	-3.359580	0.299385
106	8	4.592572	-3.259232	-1.786173
107	1	3.601973	5.283366	-1.519038
108	1	3.474194	3.648627	-2.180566
109	15	0.701691	-0.216631	-1.170632
110	8	1.112171	1.187458	-1.957168
111	8	1.793837	-0.251777	0.036652
112	8	0.836456	-1.339080	-2.156465
113	8	-0.619534	0.012358	-0.428303
114	1	2.675589	-0.525277	-0.265325
115	1	1.036758	1.011169	-2.905654

Reference:

S1 Frisch, M.J. et. al., *Gaussian 03, Revision B.05*, Gaussian, Inc., Pittsburgh PA. **2003.**

S2 Becke, A. D. *J. Chem. Phys.* **1993**, 98, 5648.

S3 Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B.* **1988**, 37, 785.

S4 W.-C.Zhang and C.-J.Li*J. Org. Chem*., **2000**, 65, 5831.

S5 R. Samanta, S. P. Mahanta, S. Chaudhuri, P. K. Panda and A.Narahari, *Inorg. Chim.Acta.,* 2011, **372**, 281.