Anion recognition by anthracene appended *ortho*-aminomethylphenylboronic acid: a new PET based sensing mechanism

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Supporting Information

*Synthesis of (2-(((anthracen-9-ylmethyl)(methyl)amino)methyl)phenyl)boronic acid, **1**.*

Receptor **1** was prepared by a reported procedure [1]:[1]

9-[(methylamino)methyl]anthracene (120 mg, 0.54 mmol) and 2-(bromomethyl)phenylboronic acid (129 mg, 0.60 mmol) were refluxed in dry acetonitrile (75 mL) for 12 h under an atmosphere of dinitrogen. Solvent was removed under reduced pressure and the resulting yellow solid was washed three times with ethyl acetate (30 mL for each one) at room temperature. The precipitate was neutralized in an aqueous solution of 10 % $NaHCO_3$ (15 mL) and separated by filtration. The resulting solid was dried under *vacuum* to give **1** as a pale-yellow crystalline powder. Yield: 142 mg, 74 %.

^{1}H NMR (300 MHz, 25°C, DMSO-d_6) δ= 9.09 (s, 2H), 8.60 (s, 1H), 8.23-8.20 (d, *J*= 7.9 Hz, 2H), 8.09-8.07 (d, *J*= 7.1 Hz, 2H), 7.83 (d, *J*= 6.9 Hz, 1H), 7.59-7.49 (m, 7H) 4.49 (s, 2H), 3.92 (s, 2H), 2.10 (s, 3H).

[1] T. D. James, K. R. A. S. Sandanayake, R. Iguchi, and S. Shinkai, J. Am. Chem. Soc., 1995, 117 (35), 8982-8987

*Synthesis of 1-(anthracen-9-yl)-N-benzyl-N-methylmethanamine, **2***

9-[(methylamino)methyl]anthracene (50.2 mg, 0.22 mmol), benzyl bromide (42 mg, 0.25 mmol) and Cs_2CO_3 were combined in dry DMF (5 mL) in a microwave vial under an atmosphere of dinitrogen. The reaction mixture was assisted by microwave twice at 80°C for 15 min with 600 watts and 10 bar. The resulting solution was filtered through celite and solvent was removed under reduced pressure to give **2** as a yellow powder. Yield: 57.4 mg, 82%.

^{1}H NMR (300 MHz, 25°C, $CDCl_3$) δ= 8.48 (d, *J*= 9.0 Hz, 2H), 8.41 (s, 1H), 8.01 (d, *J*= 9.0 Hz, 2H), 7.54-7.43 (m, 4H), 7.38-7.30 (m, 5H), 4.51 (s, 2H), 3.70 (s, 2H), 2.23 (s, 3H).

MS (EI, *m/z*) calculated for $C_{23}H_{21}N$ $[M]^{\cdot+}$ 311, found 311.

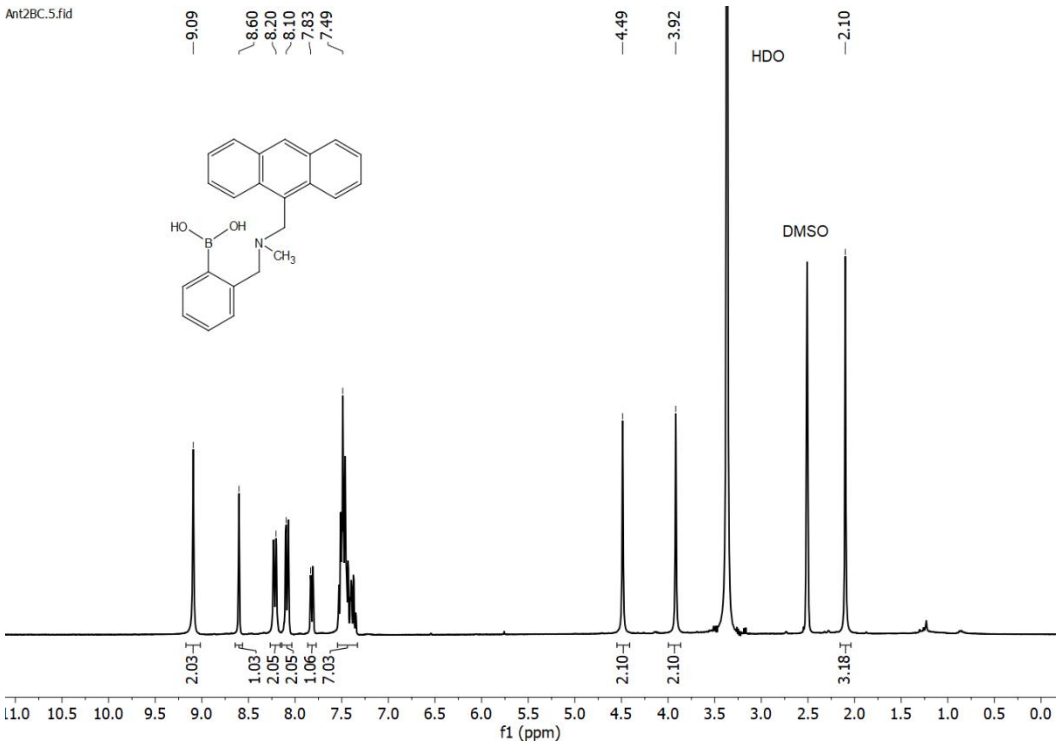


Figure S1. ^{1}H NMR spectrum of **1** in DMSO-d_6.

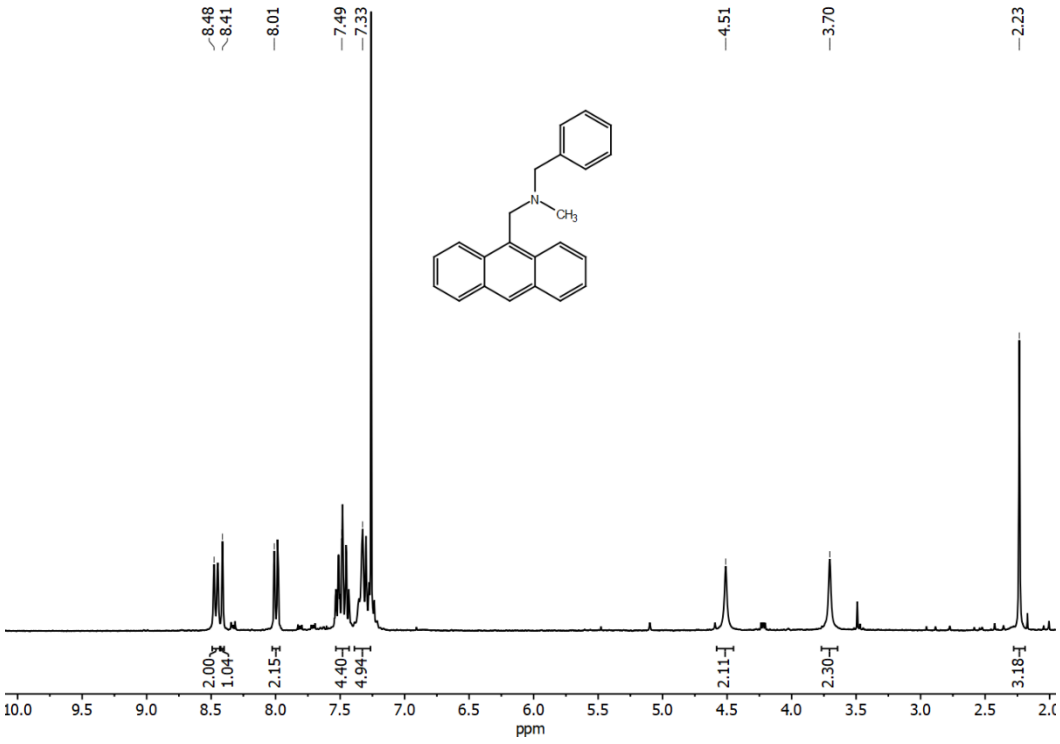


Figure S2. ^{1}H NMR spectrum of **2** in $CDCl_3$.

Table S1. Crystallographic data for compounds **1**·HBr and **2.**

	1·HBr	**2**
Empirical formula	$C_{23}H_{23}BBrNO_2$	$C_{23}H_{21}N$
Formula weight	436.14	311.41
Temperature	100(2) K	100(2) K
Wavelength	0.71073 Å	1.54178 Å
Crystal system	Triclinic	Monoclinic
Space group	P-1	$P2_1$
Unit cell dimensions	a = 8.2825(4) Å.	a = 11.90321(13) Å
	b = 9.9237(5) Å	b = 6.32633(7) Å
	c = 13.9515(6) Å	c = 12.08122(13) Å
	α= 107.3957(8)°	α= 90°
	β= 93.2715(9)°	β= 110.4706(3)°
	γ = 112.7526(8)°	γ = 90°
Volume	989.49(8) $Å^3$	852.310(16) $Å^3$
Z	2	2
P_{calcd} (g cm^{-3})	1.464	1.213
μ (mm^{-1})	2.096	0.529
Theta range for data collection	2.343 to 27.441°.	3.964 to 71.546°
Index ranges	-10<=h<=10, -12<=k<=12,	-14<=h<=14, -6<=k<=7,
	-18<=l<=18	-14<=l<=14
Reflections collected	19093	13723
Independent reflections	4525 [R(int) = 0.0224]	2972 [R(int) = 0.0252]
Data / restraints / parameters	4525 / 3 / 263	2972 / 1 / 218
Goodness-of-fit on F^2	1.131	1.057
Final R indices [I>2sigma(I)]	R1 = 0.0322, wR2 = 0.0784	R1 = 0.0279, wR2 = 0.0765
R indices (all data)	R1 = 0.0345, wR2 = 0.0794	R1 = 0.0280, wR2 = 0.0766
Largest diff. peak and hole	0.744 and -0.478 e.$Å^{-3}$	0.153 and -0.155 e.$Å^{-3}$

Table S2. Hydrogen bonds for **1**·HBr [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1O)...Br(1)	0.831(10)	2.377(13)	3.1837(15)	164(3)
O(2)-H(2O)...Br(1)#1	0.843(10)	2.438(14)	3.2499(16)	162(3)
N(1)-H(1N)...O(1)	0.891(10)	1.974(19)	2.705(2)	138(2)

Symmetry transformations used to generate equivalent atoms:
#1 -x+2,-y+2,-z+2

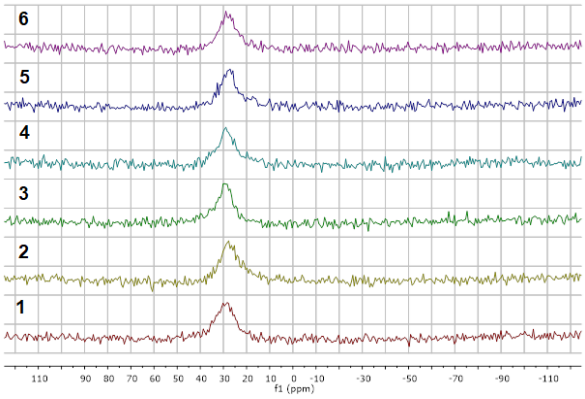


Figure S3. ^{11}B NMR titration of 11.2 mM **1** in DMSO-d_6 by acetate. Spectra 1 to 6 are recorded in the presence of 0, 5, 10, 19, 27 and 35 mM $(Bu_4N)OAc$.

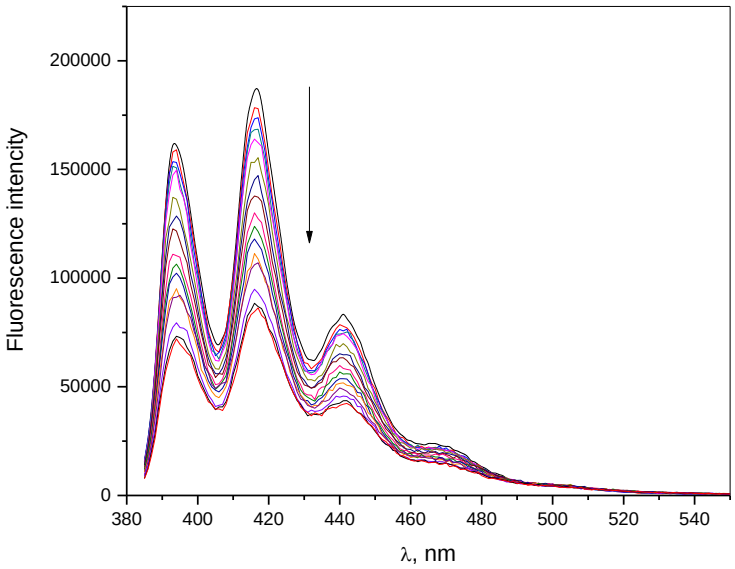


Figure S4. The course of the fluorescence titration of 10 μM **1** in DMSO by 0.2 – 80 mM $H_2PO_4^-$, excitation wavelength 370nm

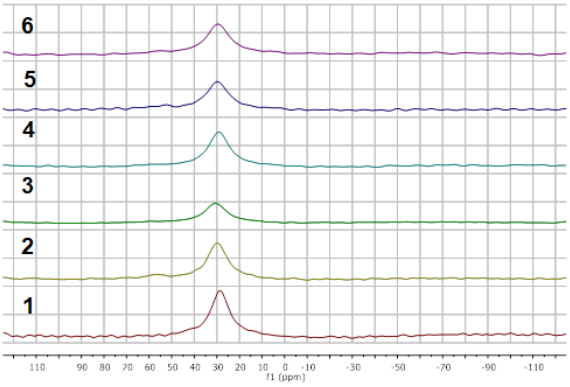


Figure S5. ^{11}B NMR titration of 19.3 mM **1** in DMSO-d_6 by dihydrogen phosphate. Spectra 1 to 6 are recorded in the presence of 0, 10.9, 21.1, 40.3, 57.5 and 73.1 mM $(Bu_4N)H_2PO_4$.

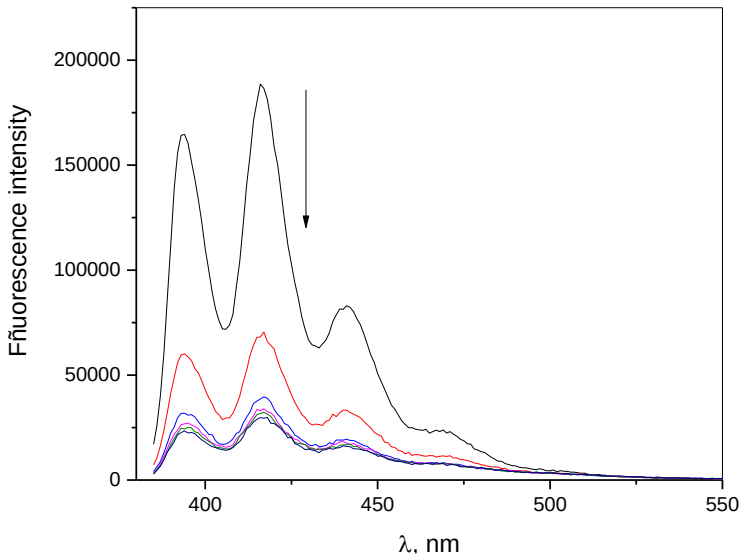


Figure S6. The course of the fluorescence titration of 10 μM **1** in DMSO by 0.25 – 1.2 mM F^-, excitation wavelength 370nm.

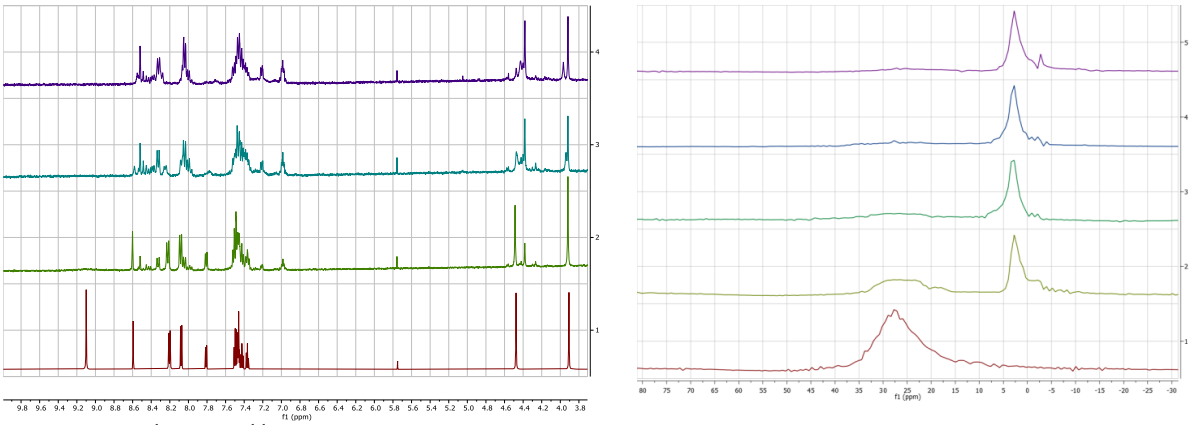


Figure S7. ^{1}H and ^{11}B NMR titration of 1.3 mM and 17.7 mM **1** respectively by $(Bu_4N)_2F$ in DMSO-d_6 Sectra from bottom to top contain 0, 0.7; 1.3 and 2 mM of $(Bu_4N)_2F$ in ^{1}H titration and 0, 8, 15.5, 30, 44 and 57 mM of $(Bu_4N)_2F$ in ^{11}B titration.

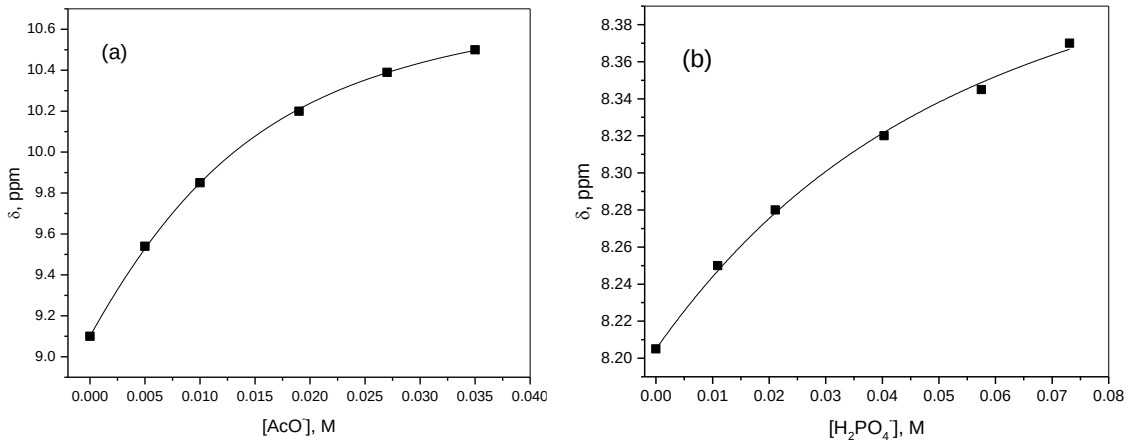


Figure S8. ^{1}H NMR titration profiles of (a) 11.2 mM **1** by acetate and (b) 19.3 mM **1** by dihydrogen phosphate in DMSO-d6; shifts of B-OH protons for acetate and of aromatic protons for dihydrogen phosphate.

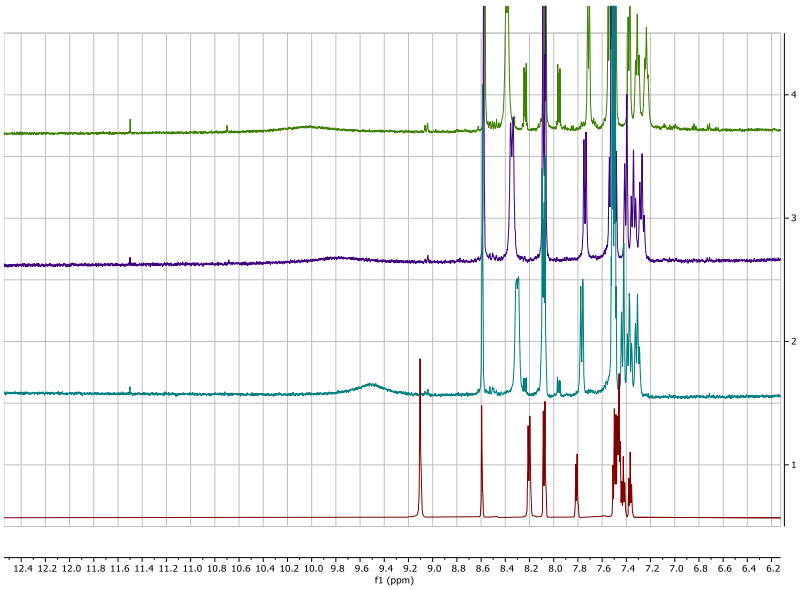
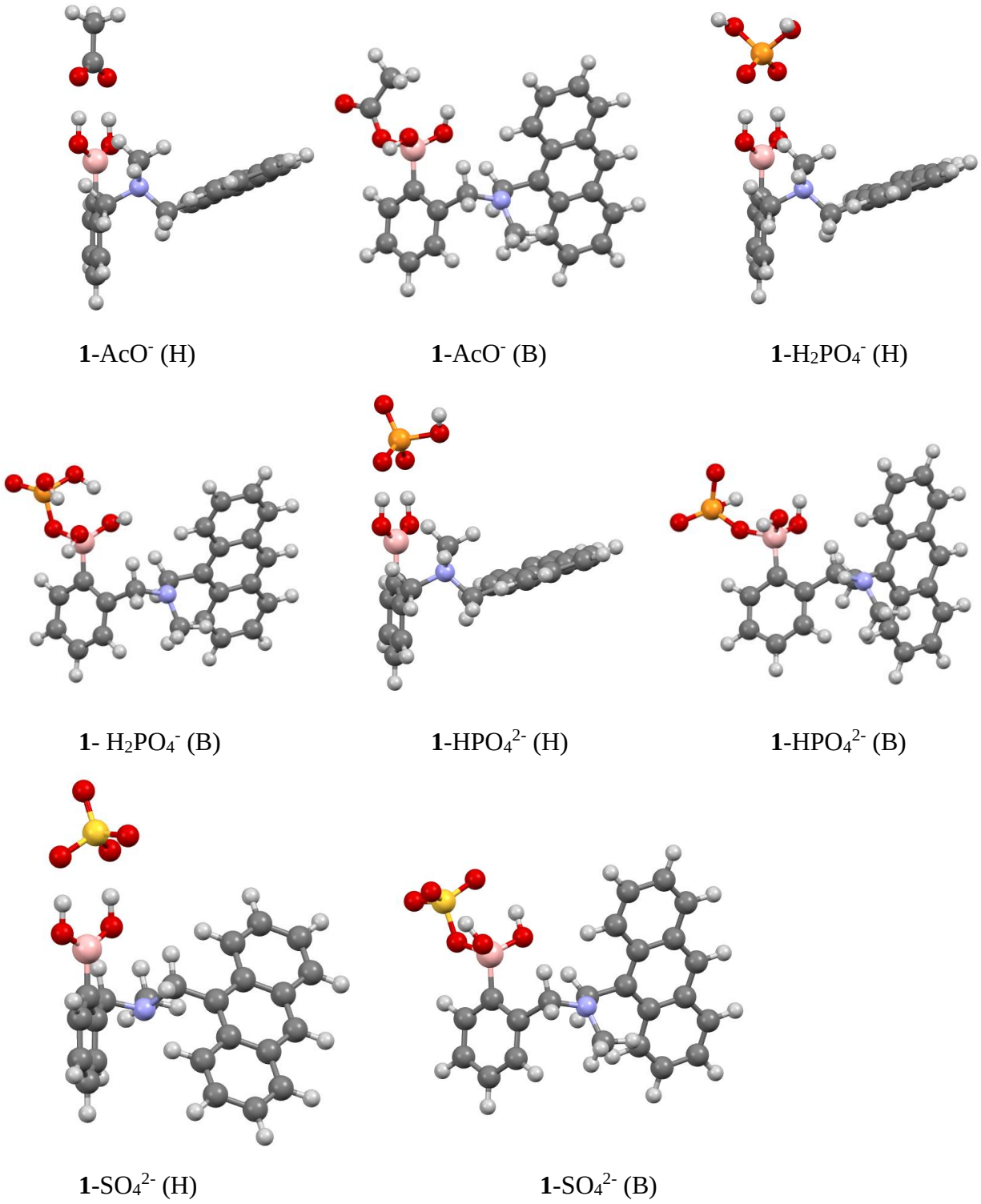


Figure S9. ^{1}H NMR titration of 3 mM **1** by $(Bu_4N)_2SO_4$. Spectra from bottom to top contain 0; 1.5; 3.0 and 4.5 mM of $(Bu_4N)_2SO_4$.

Table S3. Results of the fluorescence titrations of 0.01 mM **1** in MeCN.

Anion	K_A, M^{-1}	I_C/I_0
AcO^-	470	0.12
$H_2PO_4^-$	74	0.25
BzO^-	154	0.39
F^-	3.3×10^4	0.07
HSO_4^-	3.1×10^3	2.27



1-AcO^- (H) **1**-AcO^- (B) **1**-$H_2PO_4^-$ (H)

1- $H_2PO_4^-$ (B) **1**-HPO_4^{2-} (H) **1**-HPO_4^{2-} (B)

1-SO_4^{2-} (H) **1**-SO_4^{2-} (B)

Fig. S10. Calculated structures of H-bound (H) or B-bound (B) anion complexes of **1**.

Table S4. Sum of electronic and thermal free energies, Hartree Eh (1 Eh = 627.509 kcal/mol) and the number of imaginary frequencies for calculated structures shown in Fig. S10.

Anion	**Binding type**	**Energy**	Number of imaginary frequencies
AcO^-	B	-1348.08936	0
	H	-1348.11046	0
$H_2PO_4^-$	B	-1763.27041	0
	H	-1763.27913	0
HPO_4^{2-}	B	-1762.792521	0
	H	-1762.795419	0
SO_4^{2-}	B	-1818.91203	0
	H	-1818.920523	0

Table S5. Cartesian coordinates.

Complex **1**-AcO^- (H):

Atom	X	Y	Z
C	-2.50730	1.71428	-0.31360
C	-1.62313	2.25600	-1.26361
C	-1.35567	3.62127	-1.26827
H	-0.66169	4.02208	-1.99973
C	-1.95240	4.47248	-0.34367
H	-1.73235	5.53307	-0.36118
C	-2.81827	3.95063	0.60548
H	-3.28360	4.60134	1.33616
C	-3.08234	2.58427	0.61514
H	-3.75333	2.18013	1.36520
C	-0.90592	1.34491	-2.23023
H	-1.63351	0.71311	-2.73584
H	-0.38264	1.94179	-2.99331
C	0.32343	-0.71178	-2.34072
H	0.77167	-0.44728	-3.31205
H	-0.60267	-1.25853	-2.52092
H	1.01559	-1.37016	-1.81410
C	1.25179	1.19382	-1.18689
H	0.95391	2.14795	-0.74989
H	1.81212	1.44639	-2.09536
C	2.12556	0.46240	-0.19398
C	1.75345	0.46689	1.16502
C	0.56822	1.12011	1.63471
H	-0.08609	1.61320	0.92874
C	0.23531	1.11728	2.95357
H	-0.66995	1.61540	3.27940
C	1.05622	0.46167	3.91360

H	0.77120	0.47219	4.95810
C	2.18810	-0.17302	3.51403
H	2.82658	-0.67890	4.22917
C	2.57153	-0.19347	2.13772
C	3.73242	-0.84215	1.73080
H	4.35223	-1.34022	2.46870
C	4.11022	-0.86609	0.39431
C	5.30082	-1.54684	-0.00980
H	5.89487	-2.03051	0.75709
C	5.67357	-1.59054	-1.31350
H	6.57543	-2.11004	-1.61186
C	4.86958	-0.95159	-2.29956
H	5.16931	-0.99788	-3.33918
C	3.73375	-0.28909	-1.95490
H	3.14761	0.17543	-2.73412
C	3.29762	-0.20783	-0.59063
N	0.03108	0.46005	-1.53200
O	-3.08087	-0.53321	-1.38257
O	-3.07197	-0.35136	1.00758
B	-2.88612	0.16882	-0.23469
H	-3.33228	-1.49445	-1.24497
H	-3.35024	-1.31379	1.01998
H	-4.82552	-5.20449	1.04164
C	-4.21458	-5.00525	0.16276
H	-4.71106	-5.37019	-0.73452
C	-3.89552	-3.52406	0.04797
O	-3.79539	-2.87463	1.11713
O	-3.72653	-3.05915	-1.10593
H	-3.27323	-5.54900	0.27614

Complex **1**-AcO^- (B):

Atom	X	Y	Z
C	2.83776	-1.10526	-0.17384
C	1.92571	-1.63202	-1.11437
C	1.82939	-3.01320	-1.30645
H	1.17285	-3.39685	-2.07905
C	2.57189	-3.90581	-0.54520
H	2.48038	-4.97286	-0.71024
C	3.43684	-3.40912	0.41889
H	4.02333	-4.08731	1.02831
C	3.56868	-2.03398	0.57952
H	4.27706	-1.66082	1.30854
C	1.01409	-0.73592	-1.93760
H	1.34747	0.29490	-1.83468
H	1.08838	-1.00836	-2.99392
C	-1.12984	-1.95213	-2.06280
H	-0.90323	-2.86351	-1.49041
H	-0.89195	-2.13415	-3.11212
H	-2.20570	-1.77704	-1.98401

C	-0.66241	-0.53859	-0.17178
H	0.08411	0.17348	0.17981
H	-0.50848	-1.45141	0.41481
C	-2.04467	0.02767	0.06766
C	-2.27850	1.37581	-0.26868
C	-1.25921	2.20856	-0.83524
H	-0.27649	1.79445	-1.01620
C	-1.50602	3.50864	-1.15044
H	-0.71923	4.11850	-1.57722
C	-2.78887	4.08382	-0.92677
H	-2.96204	5.12104	-1.18505
C	-3.78459	3.33173	-0.39130
H	-4.76737	3.75280	-0.21257
C	-3.56596	1.96185	-0.04843
C	-4.58614	1.18976	0.49835
H	-5.56064	1.63511	0.66818
C	-4.37894	-0.14449	0.82456
C	-5.44058	-0.93128	1.37141
H	-6.39872	-0.45062	1.53290
C	-5.25653	-2.24073	1.67476
H	-6.06626	-2.82988	2.08658
C	-3.98946	-2.84866	1.44505
H	-3.85416	-3.89703	1.68053
C	-2.95278	-2.13317	0.93415
H	-2.00887	-2.63162	0.76797
C	-3.09154	-0.74380	0.60355
N	-0.41438	-0.78066	-1.59256
O	3.61214	1.07902	-1.31801
O	1.97974	1.25502	0.39002
B	3.14408	0.51050	-0.05316
H	4.34428	0.56658	-1.67089
H	2.02721	2.15726	0.05966
H	3.39169	3.22824	1.58336
O	5.76526	1.59390	2.26819
C	4.84377	1.67407	1.47197
C	4.32270	3.02866	1.04943
O	4.27902	0.60334	0.98888
H	4.11864	3.05558	-0.01931
H	5.05013	3.79091	1.31774

Complex **1**-$H_2PO_4^-$ (H):

Atom	X	Y	Z
C	-1.66481	2.48449	-0.32873
C	-0.68402	2.80715	-1.28354
C	-0.11524	4.07658	-1.29642
H	0.65042	4.30582	-2.03011
C	-0.50395	5.04612	-0.37743
H	-0.05051	6.02967	-0.40158
C	-1.46449	4.73929	0.57432

H	-1.77113	5.48295	1.30002
C	-2.02875	3.46719	0.59393
H	-2.77227	3.22991	1.34690
C	-0.19573	1.75232	-2.24692
H	-1.04847	1.31165	-2.75959
H	0.45869	2.20823	-3.00576
C	0.49716	-0.54381	-2.34098
H	0.99180	-0.40456	-3.31569
H	-0.53414	-0.85316	-2.51368
H	1.01192	-1.34477	-1.80877
C	1.86314	1.09048	-1.20496
H	1.80670	2.09340	-0.77926
H	2.46663	1.18901	-2.11551
C	2.53665	0.18008	-0.20446
C	2.18936	0.29654	1.15610
C	1.20361	1.22622	1.62061
H	0.68214	1.85279	0.90993
C	0.89270	1.32485	2.94120
H	0.13887	2.03315	3.26343
C	1.53862	0.50435	3.90806
H	1.27492	0.60065	4.95380
C	2.47748	-0.39364	3.51344
H	2.97986	-1.02883	4.23395
C	2.83060	-0.52879	2.13557
C	3.79331	-1.44831	1.73340
H	4.27999	-2.07089	2.47654
C	4.13954	-1.58631	0.39522
C	5.12190	-2.54556	-0.00371
H	5.58771	-3.14751	0.76805
C	5.45778	-2.70153	-1.30881
H	6.20085	-3.43174	-1.60352
C	4.82424	-1.90134	-2.30146
H	5.09106	-2.03811	-3.34211
C	3.89046	-0.97355	-1.96209
H	3.42699	-0.39355	-2.74676
C	3.50322	-0.76455	-0.59648
N	0.49999	0.67136	-1.54290
O	-2.74902	0.44259	-1.39159
O	-2.64417	0.60133	1.01032
B	-2.37843	1.06451	-0.23977
H	-3.18901	-0.44015	-1.30292
H	-3.14461	-0.25051	1.08195
H	-6.20179	-3.03510	-0.76036
O	-5.88286	-2.76966	0.11150
P	-4.30023	-2.46997	0.09318
O	-4.00008	-1.67106	1.31052
O	-3.91750	-1.95257	-1.25710
O	-3.63304	-3.92318	0.29311
H	-3.44408	-4.34012	-0.55678

Complex **1**-$H_2PO_4^-$ (B):

Atom	X	Y	Z
C	-2.34077	1.49995	-0.35003
C	-1.34308	1.92392	-1.25257
C	-1.08729	3.28794	-1.42199
H	-0.36706	3.60321	-2.16771
C	-1.74976	4.24985	-0.67315
H	-1.53281	5.30097	-0.82116
C	-2.69783	3.84668	0.25605
H	-3.22424	4.58108	0.85452
C	-2.99037	2.49540	0.39217
H	-3.76114	2.19704	1.09170
C	-0.50114	0.94769	-2.06066
H	-0.94005	-0.04895	-2.00668
H	-0.50903	1.24550	-3.11216
C	1.75562	1.94124	-2.06341
H	1.60361	2.84650	-1.45865
H	1.57170	2.18864	-3.10994
H	2.80391	1.65118	-1.96151
C	1.07495	0.50991	-0.25175
H	0.29267	-0.19500	0.03005
H	0.91153	1.39295	0.37557
C	2.42297	-0.11224	0.03842
C	2.65068	-1.43876	-0.37685
C	1.67051	-2.19459	-1.09821
H	0.73476	-1.72610	-1.37042
C	1.90643	-3.47971	-1.47603
H	1.14946	-4.02830	-2.02278
C	3.14170	-4.11611	-1.16751
H	3.30720	-5.14036	-1.47717
C	4.10371	-3.43549	-0.49316
H	5.05213	-3.90186	-0.25230
C	3.89441	-2.08340	-0.08106
C	4.88163	-1.38528	0.60671
H	5.82232	-1.87551	0.83375
C	4.68526	-0.06807	1.00174
C	5.71690	0.64351	1.69005
H	6.64209	0.11949	1.90103
C	5.54556	1.93649	2.06339
H	6.33255	2.46910	2.58230
C	4.32243	2.60177	1.76599
H	4.19800	3.63732	2.05745
C	3.31331	1.95714	1.12241
H	2.40388	2.49980	0.90937
C	3.43972	0.58789	0.71275
N	0.90833	0.83064	-1.66721
O	-3.35834	-0.55712	-1.52938
O	-1.88558	-1.04297	0.25925
B	-2.86042	-0.04623	-0.23072

H	-3.68670	0.15514	-2.08642
H	-1.51229	-1.52671	-0.48486
O	-3.99954	-0.05842	0.77636
H	-4.57971	-1.63613	-0.93030
O	-5.14321	-2.03140	-0.22052
P	-4.75358	-1.36142	1.16751
O	-5.91097	-1.20835	2.05367
O	-3.64786	-2.30007	1.81812
H	-2.79453	-2.07905	1.37787

Complex **1**-HPO_4^{2-} (H):

Atom	X	Y	Z
C	-1.88867	2.37046	-0.32783
C	-0.91255	2.71890	-1.27962
C	-0.38208	4.00546	-1.30145
H	0.37850	4.25224	-2.03523
C	-0.80307	4.97119	-0.39261
H	-0.38031	5.96824	-0.42347
C	-1.75834	4.64151	0.55728
H	-2.09116	5.38136	1.27574
C	-2.28360	3.35240	0.58349
H	-3.02230	3.09684	1.33556
C	-0.38726	1.67306	-2.23359
H	-1.22821	1.17575	-2.71193
H	0.22667	2.14730	-3.01555
C	0.42550	-0.58518	-2.29826
H	0.88913	-0.44136	-3.28794
H	-0.59178	-0.95263	-2.43718
H	0.99597	-1.34539	-1.76246
C	1.72450	1.14014	-1.22082
H	1.62233	2.14544	-0.80859
H	2.30764	1.25537	-2.14287
C	2.45988	0.28364	-0.21620
C	2.10505	0.38601	1.14326
C	1.05486	1.24709	1.59782
H	0.49124	1.82737	0.88007
C	0.73290	1.33184	2.91661
H	-0.07152	1.98563	3.23172
C	1.43305	0.56631	3.89094
H	1.15918	0.65001	4.93517
C	2.43539	-0.26471	3.50554
H	2.97932	-0.85731	4.23217
C	2.80099	-0.38461	2.12947
C	3.82665	-1.23690	1.73488
H	4.35622	-1.81708	2.48303
C	4.18054	-1.36259	0.39740
C	5.22731	-2.25422	0.00543
H	5.73663	-2.81308	0.78215
C	5.56955	-2.40099	-1.29914

H	6.36172	-3.08012	-1.58807
C	4.87699	-1.66053	-2.29871
H	5.14805	-1.79208	-3.33893
C	3.88181	-0.79622	-1.96603
H	3.37422	-0.26056	-2.75494
C	3.48685	-0.59745	-0.60123
N	0.38097	0.64495	-1.52603
O	-2.89028	0.27906	-1.38103
O	-2.83751	0.46996	1.01797
B	-2.56886	0.92033	-0.23246
H	-3.30626	-0.67056	-1.29125
H	-3.33895	-0.43275	1.07149
O	-5.28054	-3.66853	0.07211
P	-4.12250	-2.71144	0.07357
O	-4.09047	-1.70990	1.22267
O	-3.87884	-2.02646	-1.27411
O	-2.76920	-3.63080	0.35610
H	-2.84416	-4.44150	-0.15716

Complex **1**-HPO_4^{2-} (B):

Atom	X	Y	Z
C	-2.34742	1.54770	-0.31876
C	-1.34212	2.01525	-1.19060
C	-1.08201	3.38494	-1.30036
H	-0.35460	3.73185	-2.02562
C	-1.75112	4.31561	-0.51640
H	-1.53260	5.37237	-0.61587
C	-2.70840	3.87076	0.38472
H	-3.24027	4.57946	1.00983
C	-3.00091	2.51313	0.45877
H	-3.77911	2.17740	1.13410
C	-0.50595	1.06219	-2.02933
H	-0.95920	0.07235	-1.99144
H	-0.51349	1.38618	-3.07369
C	1.76452	2.03011	-2.03442
H	1.62338	2.93354	-1.42351
H	1.58294	2.28710	-3.07926
H	2.81070	1.72972	-1.93561
C	1.07552	0.59691	-0.22987
H	0.25377	-0.05773	0.06380
H	0.97721	1.49076	0.39629
C	2.39053	-0.10221	0.03647
C	2.52804	-1.44216	-0.37641
C	1.48405	-2.13885	-1.06678
H	0.56889	-1.61587	-1.30700
C	1.63178	-3.43648	-1.44670
H	0.82780	-3.94012	-1.96904
C	2.83484	-4.14530	-1.16989
H	2.92986	-5.17836	-1.48009

C	3.85417	-3.52292	-0.52377
H	4.77875	-4.04545	-0.30647
C	3.73807	-2.15976	-0.11129
C	4.78360	-1.52025	0.54682
H	5.69925	-2.06497	0.75083
C	4.67659	-0.19248	0.94076
C	5.76703	0.45864	1.59793
H	6.66463	-0.11899	1.78701
C	5.68368	1.76088	1.96894
H	6.51502	2.24700	2.46380
C	4.49491	2.49759	1.70107
H	4.44039	3.53965	1.99081
C	3.43229	1.91224	1.08781
H	2.55094	2.50676	0.89655
C	3.46537	0.53658	0.68108
N	0.90652	0.92699	-1.64365
O	-3.25562	-0.46571	-1.59281
O	-1.80531	-0.94671	0.28704
B	-2.86730	-0.01774	-0.25868
H	-3.92067	-1.15942	-1.43701
H	-1.58936	-1.55784	-0.42390
O	-4.02393	-0.06739	0.68467
O	-5.00823	-2.19284	-0.24154
P	-4.76975	-1.42774	1.03507
O	-5.92900	-1.17512	1.93496
O	-3.63033	-2.20151	1.90543
H	-2.78024	-1.95787	1.48758

Complex **1**-SO_4^{2-} (H):

Atom	X	Y	Z
C	-1.72909	2.33831	0.41815
C	-0.61677	2.36392	1.27316
C	0.20580	3.49346	1.31278
H	1.05468	3.49709	1.98885
C	-0.03488	4.59192	0.50467
H	0.62018	5.45398	0.54685
C	-1.12975	4.57945	-0.35340
H	-1.33442	5.43143	-0.99074
C	-1.96284	3.47200	-0.37665
H	-2.82585	3.47108	-1.03233
C	-0.24702	1.22773	2.20150
H	-0.13413	1.63481	3.20952
H	-1.04104	0.47400	2.22954
C	1.52128	-0.19856	2.94757
H	0.82193	-1.01351	3.19461
H	1.65128	0.42179	3.83533
H	2.48585	-0.64151	2.69712
C	0.92213	-0.16664	0.61554
H	0.38532	0.43678	-0.11714

H	0.28865	-1.04290	0.78237
C	2.26731	-0.55799	0.04679
C	3.02782	0.41690	-0.62879
C	2.57340	1.76533	-0.79154
H	1.61882	2.05790	-0.37827
C	3.32352	2.69075	-1.44785
H	2.95442	3.70362	-1.55529
C	4.59047	2.34678	-1.99808
H	5.17073	3.09923	-2.51729
C	5.06084	1.07935	-1.87108
H	6.02160	0.79657	-2.28585
C	4.30286	0.07940	-1.18706
C	4.78529	-1.21850	-1.05907
H	5.74980	-1.47427	-1.48460
C	4.05340	-2.19277	-0.39176
C	4.56794	-3.52013	-0.25829
H	5.53247	-3.73829	-0.70232
C	3.87249	-4.47654	0.40663
H	4.26934	-5.47914	0.50462
C	2.61058	-4.15911	0.98423
H	2.06460	-4.92606	1.51953
C	2.08422	-2.91057	0.87365
H	1.12694	-2.70900	1.33142
C	2.77514	-1.86448	0.17613
N	1.04190	0.62236	1.84692
O	-2.33158	-0.14971	0.40353
O	-4.02606	1.47747	-0.09398
B	-2.75983	1.12709	0.24944
H	-3.03029	-0.86826	0.24997
H	-4.67251	0.71338	-0.23588
O	-4.90217	-1.84490	-2.18333
O	-5.75848	-0.40782	-0.42771
S	-5.26594	-1.78332	-0.76009
O	-4.05030	-2.03706	0.07984
O	-6.30170	-2.76769	-0.42679

Complex **1**-SO_4^{2-} (B):

Atom	X	Y	Z
C	-2.29409	1.56806	-0.23813
C	-1.29097	2.06096	-1.09738
C	-1.02710	3.43203	-1.16232
H	-0.29864	3.80185	-1.87519
C	-1.69588	4.33663	-0.34728
H	-1.47652	5.39593	-0.41129
C	-2.65362	3.86391	0.53924
H	-3.18413	4.55308	1.18686
C	-2.94732	2.50451	0.57261
H	-3.72305	2.15168	1.24256
C	-0.47100	1.11943	-1.96362

H	-0.93352	0.13375	-1.93584
H	-0.47874	1.46655	-3.00054
C	1.81101	2.05274	-1.98145
H	1.68435	2.95823	-1.37003
H	1.62572	2.31168	-3.02522
H	2.85455	1.74139	-1.88991
C	1.11361	0.62439	-0.17132
H	0.27000	0.00189	0.12779
H	1.06304	1.52301	0.45436
C	2.40518	-0.12612	0.06907
C	2.46446	-1.48479	-0.30121
C	1.34283	-2.16825	-0.87524
H	0.40735	-1.64027	-1.01018
C	1.42645	-3.47905	-1.23045
H	0.56442	-3.97634	-1.65816
C	2.63136	-4.21369	-1.04316
H	2.67347	-5.25563	-1.33513
C	3.71582	-3.60796	-0.49466
H	4.63995	-4.15256	-0.33790
C	3.66973	-2.23326	-0.10731
C	4.77947	-1.61265	0.45775
H	5.69104	-2.18136	0.60769
C	4.74075	-0.27469	0.82903
C	5.89146	0.35355	1.40046
H	6.78073	-0.24920	1.54531
C	5.87324	1.66498	1.74754
H	6.74930	2.13293	2.17876
C	4.69357	2.43507	1.53965
H	4.68996	3.48342	1.81128
C	3.57699	1.87318	1.00559
H	2.70391	2.49185	0.85819
C	3.53988	0.48907	0.62876
N	0.94179	0.96052	-1.58523
O	-3.33606	-0.29137	-1.59069
O	-1.70490	-0.89905	0.13818
B	-2.78724	0.00069	-0.26410
H	-4.11476	-0.85281	-1.48324
H	-2.11811	-1.69749	0.49406
O	-3.92124	-0.11903	0.77842
O	-5.46805	-1.66158	-0.28044
S	-4.74097	-1.42718	0.97173
O	-5.62365	-1.16682	2.09472
O	-3.77689	-2.49992	1.23958

Complex **1**-HOx$^-$ (**7'**):

Atom	X	Y	Z
C	-3.11112	0.86731	-0.26905
C	-2.22138	1.51019	-1.15333

C	-2.21771	2.90440	-1.24386
H	-1.57768	3.38831	-1.97178
C	-3.03437	3.68427	-0.43662
H	-3.01405	4.76392	-0.52409
C	-3.88064	3.06618	0.47267
H	-4.52210	3.65962	1.11343
C	-3.92001	1.67887	0.53616
H	-4.61146	1.20837	1.22509
C	-1.24164	0.72758	-2.01467
H	-1.49170	-0.33306	-1.97200
H	-1.33589	1.04592	-3.05598
C	0.80275	2.10606	-2.05465
H	0.51841	2.95768	-1.42042
H	0.53934	2.33923	-3.08737
H	1.88874	2.00302	-1.99599
C	0.44524	0.54070	-0.25875
H	-0.20354	-0.28549	0.02825
H	0.17345	1.37761	0.39415
C	1.88415	0.12947	-0.03803
C	2.28463	-1.15098	-0.46773
C	1.38277	-2.05968	-1.11134
H	0.35762	-1.76095	-1.28312
C	1.79236	-3.29308	-1.51290
H	1.09095	-3.96282	-1.99505
C	3.13445	-3.72059	-1.30767
H	3.43744	-4.70698	-1.63586
C	4.02368	-2.89246	-0.70192
H	5.04936	-3.20104	-0.53534
C	3.63278	-1.58907	-0.26604
C	4.54406	-0.74047	0.35422
H	5.56437	-1.07465	0.50906
C	4.17066	0.53016	0.77320
C	5.12168	1.39749	1.39606
H	6.13020	1.02698	1.53984
C	4.77441	2.64803	1.79112
H	5.50100	3.29937	2.26034
C	3.44432	3.11152	1.58274
H	3.17796	4.11461	1.89212
C	2.50876	2.31495	1.00131
H	1.51232	2.70541	0.85493
C	2.82131	0.98186	0.57276
N	0.17738	0.85626	-1.66091
O	-3.86509	-1.25451	-1.48851
B	-3.34769	-0.73972	-0.26220
H	-4.12171	-0.55290	-2.09102
O	-4.26653	-1.12452	0.89852
O	-4.12424	-2.34129	2.77693
C	-3.66515	-1.89326	1.75833
C	-2.23210	-2.15268	1.24460
O	-2.09719	-1.53273	0.10627
O	-1.40066	-2.81545	1.80785