Electronic Supplementary Material (ESI) for Dalton Transactions.

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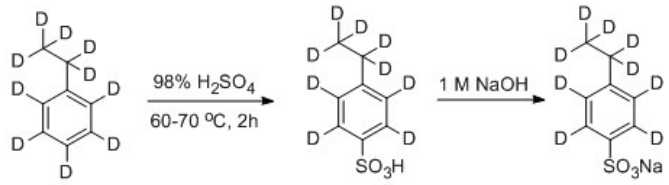
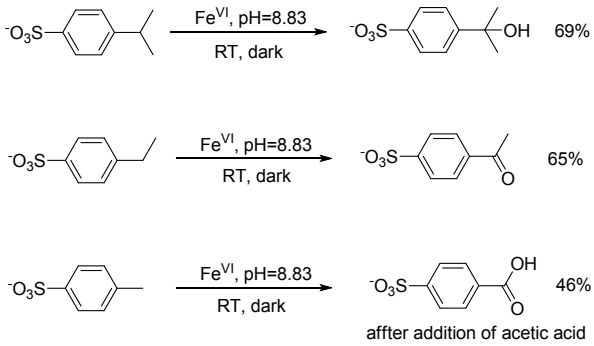
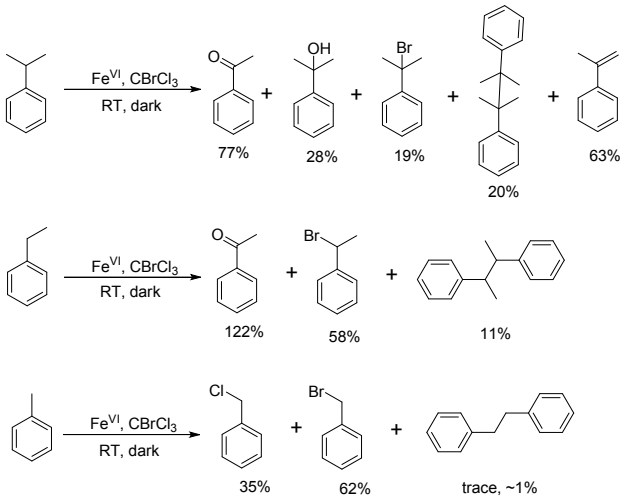
Supporting Information



Scheme S1 Synthesis of sodium 4-ethylbenzenesulfonate-d_9.



Scheme S2 Oxidation of alkylbenzenesulfonates by ferrate at pH = 8.83.



Scheme S3 The products in the organic phase for the oxidation of alkylarenes by ferrate at pH = 8.67.

Table S1 Second-order rate constants of the oxidation of 4-isopropylbenzenesulfonate by ferrate at 25 ˚C and I = 0.3 M.

pH	k_2 / M^{-1} s^{-1}
7.45	$(2.24 \pm 0.07) \times 10^{-1}$
7.83	$(1.17 \pm 0.04) \times 10^{-1}$
8.11	$(7.63 \pm 0.38) \times 10^{-2}$
8.35	$(4.18 \pm 0.17) \times 10^{-2}$
8.51	$(3.13 \pm 0.12) \times 10^{-2}$
8.83	$(1.77 \pm 0.06) \times 10^{-2}$
9.01	$(1.52 \pm 0.01) \times 10^{-2}$
9.63	$(8.51 \pm 0.18) \times 10^{-3}$

Table S2 Second-order rate constants of the oxidation of 4-isopropylbenzenesulfonate by ferrate at 25 ˚C and pH = 8.35.

I / M	k_2 / M^{-1} s^{-1}
0.15	$(3.37 \pm 0.11) \times 10^{-2}$
0.30	$(4.18 \pm 0.17) \times 10^{-2}$
0.60	$(5.03 \pm 0.15) \times 10^{-2}$
0.80	$(5.73 \pm 0.33) \times 10^{-2}$

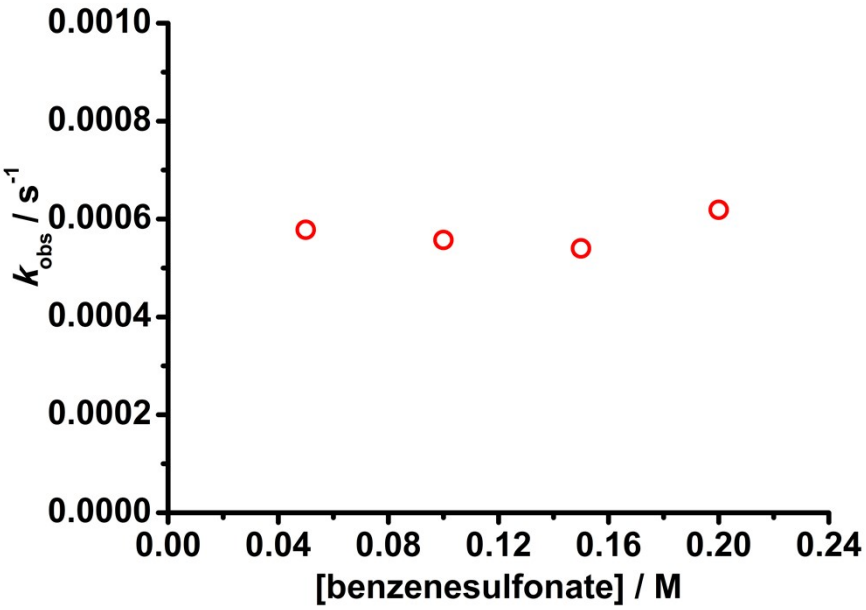


Fig. S1 Plot of k_{obs} vs [benzenesulfonate] for the oxidation of benzenesulfonate by ferrate at 25 ˚C, pH=8.83 and I = 0.3 M.

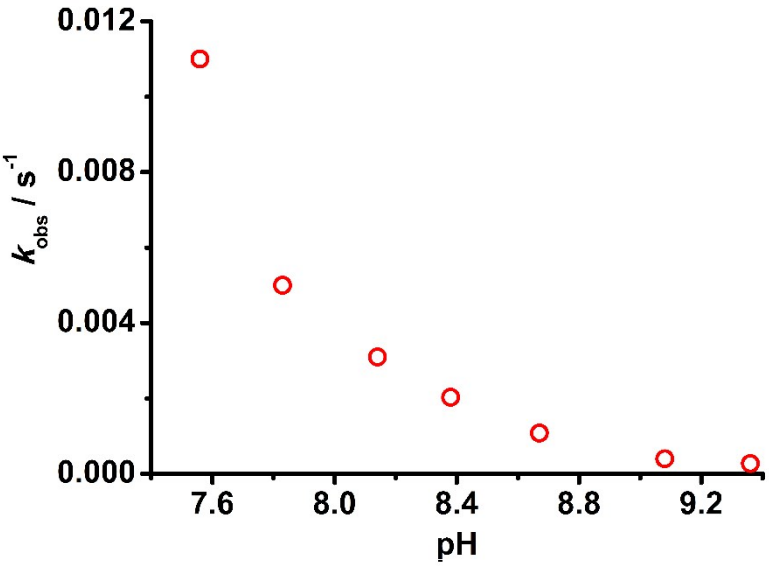


Fig. S2 Plot of k_{obs} vs. pH for the self-decomposition of ferrate(VI) at I = 0.3 M and 25 °C.

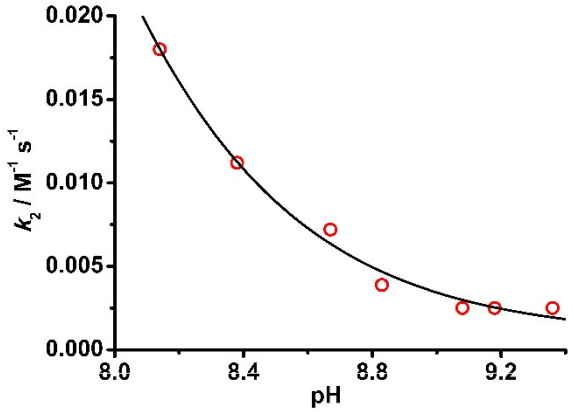


Fig. S3 Plot of k_2 vs. pH for the oxidation of 4-methylbenzenesulfonate by ferrate(VI) at I = 0.3 M and 25 °C. The solid line represents the fit of the experimental data according to eqn (7).

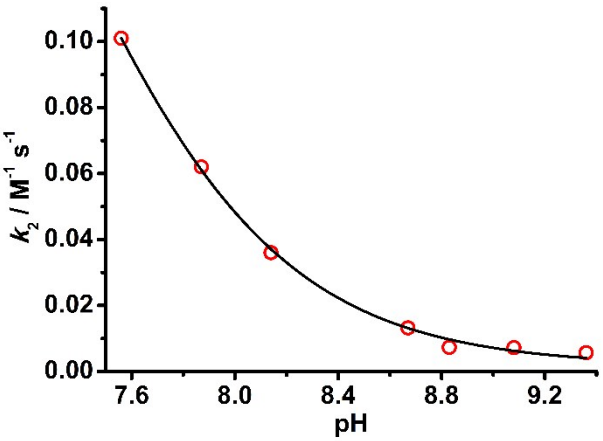


Fig. S4 Plot of k_2 vs. pH for the oxidation of 4-ethylbenzenesulfonate by ferrate(VI) at I = 0.3 M and 25 °C. The solid line represents the fit of the experimental data according to eqn (7).

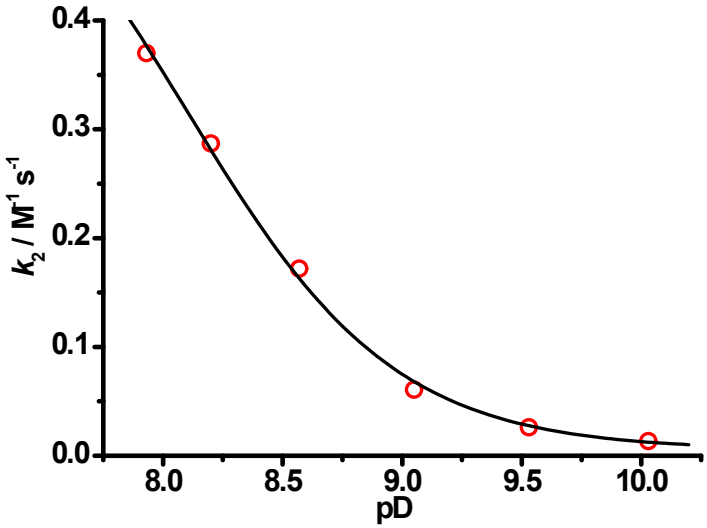


Fig. S5 Plot of k_2 vs. pD for the oxidation of 4-isopropylbenzenesulfonate by ferrate(VI) in D_2O at I = 0.3 M and 25 °C. The solid line represents the fit of the experimental data according to eqn 7.

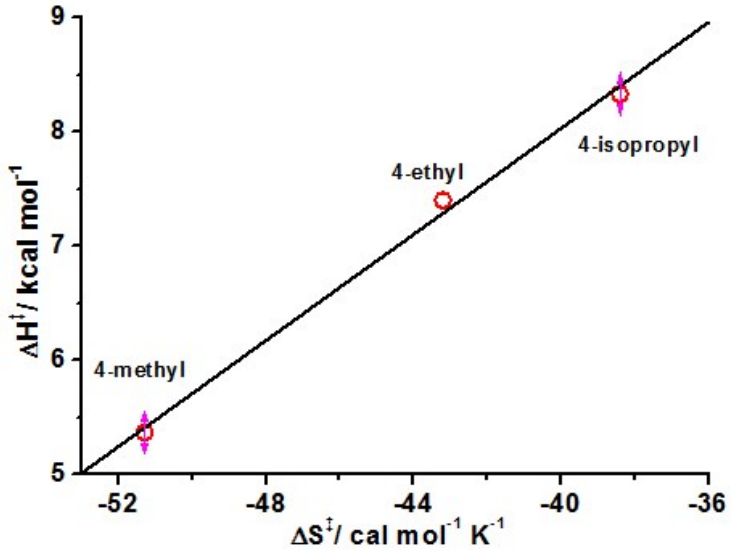


Fig. S6 Plot of $\Delta H^{\ddagger}$ versus $\Delta S^{\ddagger}$ for the oxidation of alkylbenzenesulfonates by ferrate at pH=8.83 and I = 0.3 M [slope = 0.23 ± 0.02; y-intercept = (1.73 ± 0.07) × 10^1; r^2 = 0.992]

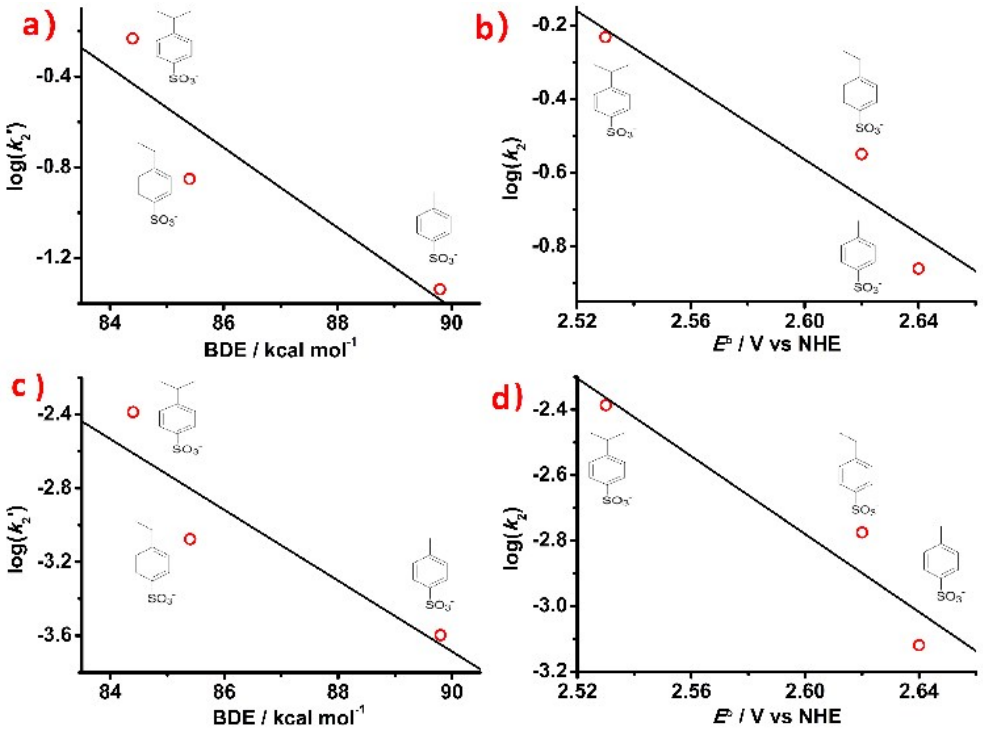


Fig. S7 a) Plot of logk_2' vs BDEs of alkyl benzenesulfonates for the reactions with $[Fe(O)_3(OH)]^-$ [slope = – (0.17 ± 0.07); *y*-intercept = (14.4 ± 6.7)]. b) Plot of logk_2 vs E^0 of alkylbenzenesulfonates for the reactions with $[Fe(O)_3(OH)]^-$ [slope = – (5.04 ± 1.81); *y*-intercept = (12.5 ± 4.7)]. c) Plot of logk_2' vs BDEs of alkylbenzenesulfonates for the reactions with $[FeO_4]^{2-}$ [slope = – (0.19 ± 0.09); *y*-intercept = (13.6 ± 7.6)]. d) Plot of logk_2 vs E^0 of alkyl benzenesulfonates for the reactions with $[FeO_4]^{2-}$ [slope = – (5.96 ± 1.95); *y*-intercept = (12.7 ± 5.1)].

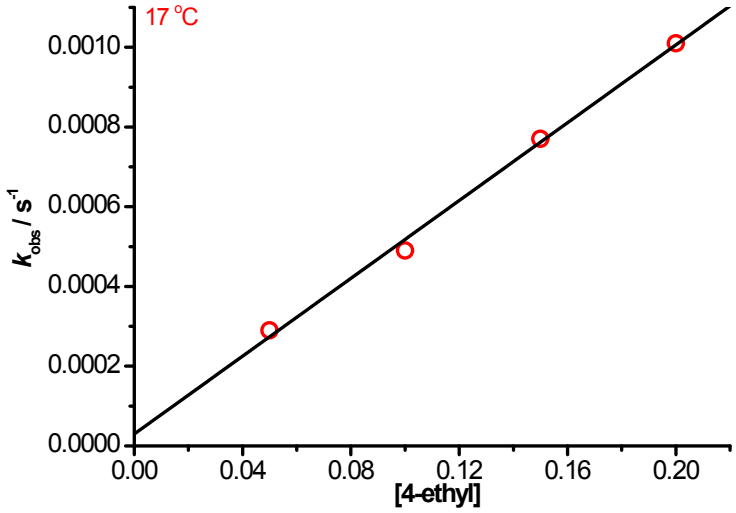


Fig. S8 Plot of k_{obs} vs [4-ethyl] for the oxidation of 4-ethylbenzenesulfonate by ferrate at 17 ˚C, pH=8.83 and I = 0.3 M [slope = (4.88 ± 0.21) × 10^{-3}; y-intercept = (3.00 ±2.89) × 10^{-5}; r^2 = 0.998]

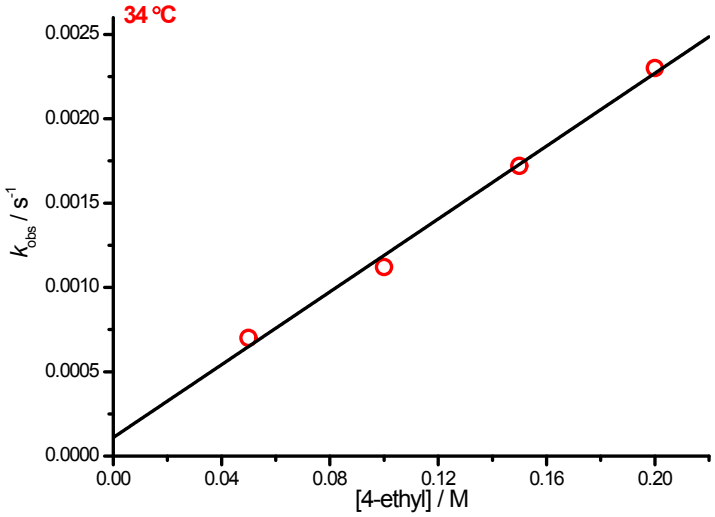


Fig. S9 Plot of k_{obs} vs [4-ethyl] for the oxidation of 4-ethylbenzenesulfonate by ferrate at 34 ˚C, pH=8.83 and I = 0.3 M [slope = (1.08 ± 0.06) × 10^{-2}; y-intercept = (1.10 ±0.79) × 10^{-4}; r^2 = 0.998].

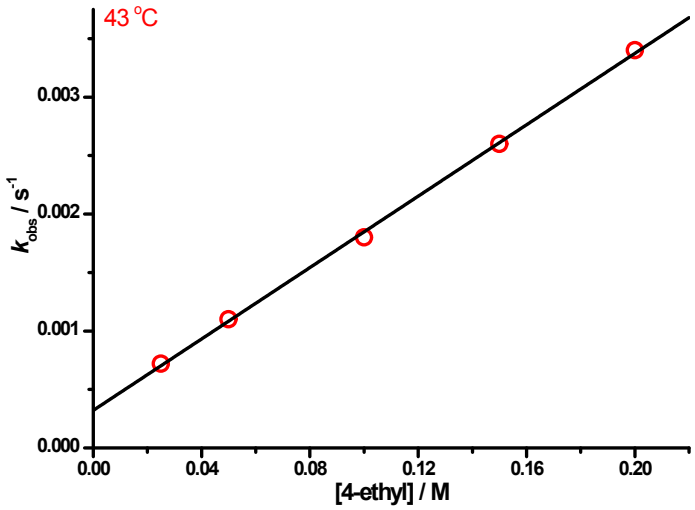


Fig. S10 Plot of k_{obs} vs [4-ethyl] for the oxidation of 4-ethylbenzenesulfonat by ferrate at 43 ˚C, pH=8.83 and I = 0.3 M [slope = (1.53 ± 0.02) × 10^{-2}; y-intercept = (3.21 ±0.30) × 10^{-4}; r^2 = 0.999].

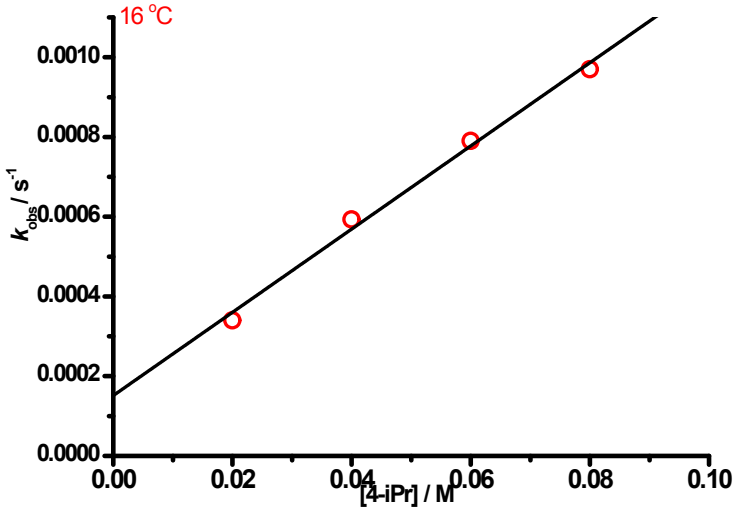


Fig. S11 Plot of k_{obs} vs [4-isopropyl] for the oxidation of 4-isopropylbenzenesulfonate by ferrate at 16 ˚C, pH=8.83 and I = 0.3 M [slope = (1.04 ± 0.06) × 10^{-2}; y-intercept = (1.52 ±0.32) × 10^{-4}; r^2 = 0.997].

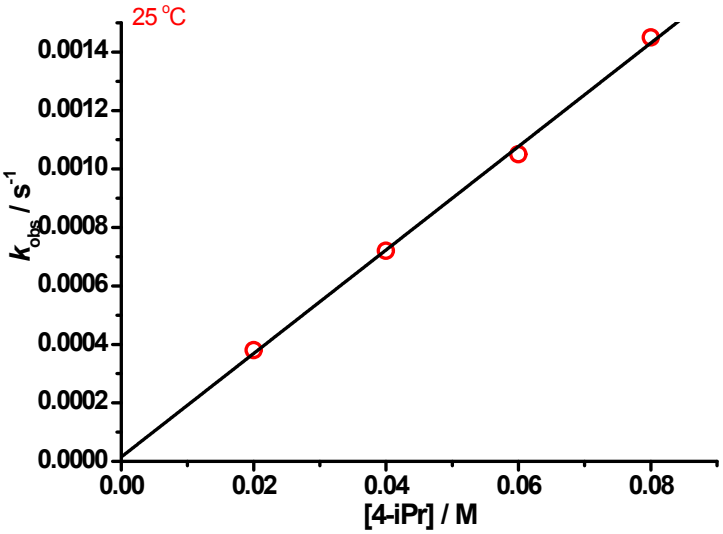


Fig. S12 Plot of k_{obs} vs [4-isopropyl] for the oxidation of 4-isopropylbenzenesulfonate by ferrate at 25 °C, pH=8.83 and I = 0.3 M [slope = (1.77 ± 0.06) × 10^{-2}; y-intercept = (1.50 ± 3.02) × 10^{-5}; r^2 = 0.999].

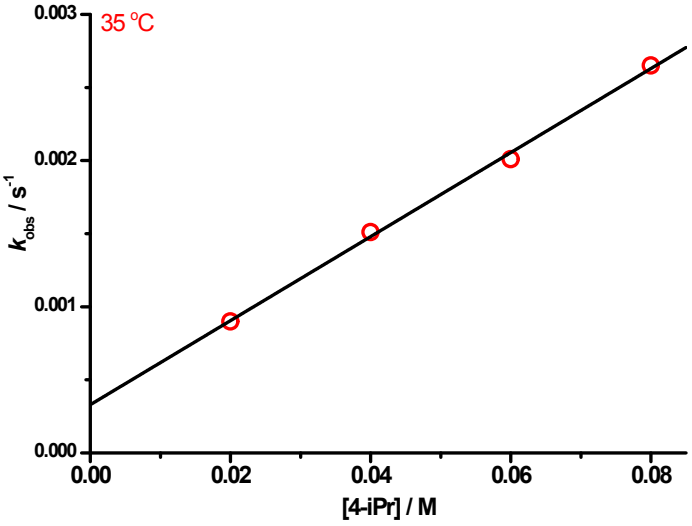


Fig. S13 Plot of k_{obs} vs [4-isopropyl] for the oxidation of 4-isopropylbenzenesulfonate by ferrate at 35 °C, pH=8.83 and I = 0.3 M [slope = (2.88 ± 0.09) × 10^{-2}; y-intercept = (3.30 ±0.50) × 10^{-4}; r^2 = 0.999].

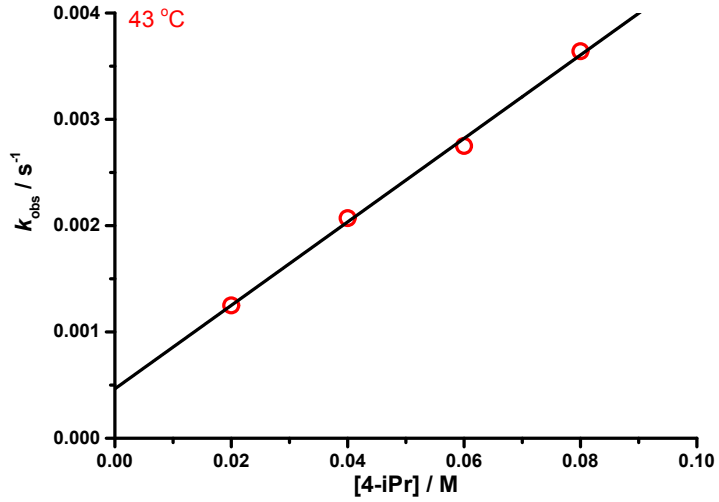


Fig. S14 Plot of k_{obs} vs [4-isopropyl] for the oxidation of 4-isopropylbenzenesulfonate by ferrate at 35 ˚C, pH=8.83 and I = 0.3 M [slope = (2.88 ± 0.09) × 10^{-2}; y-intercept = (3.30 ±0.50) × 10^{-4}; r^2 = 0.999].

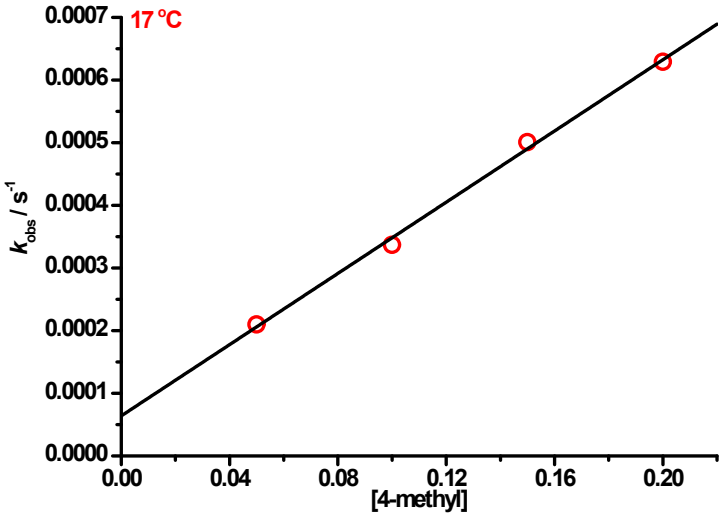


Fig. S15 Plot of k_{obs} vs [4-methyl] for the oxidation of 4-methylbenzenesulfonate by ferrate at 17 ˚C, pH=8.83 and I = 0.3 M [slope = (2.84 ± 0.10) × 10^{-3}; y-intercept = (6.40 ± 1.41) × 10^{-5}; r^2 = 0.999].

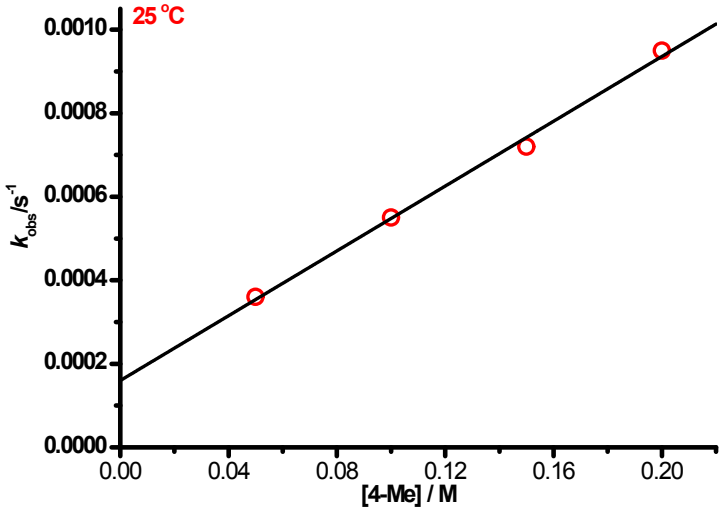


Fig. S16 Plot of k_{obs} vs [4-methyl] for the oxidation of 4-methylbenzenesulfonate by ferrate at 25 ˚C, pH=8.83 and I = 0.3 M [slope = (3.88 ± 0.17) × 10^{-3}; y-intercept = (1.60 ± 0.23) × 10^{-4}; r^2 = 0.998].

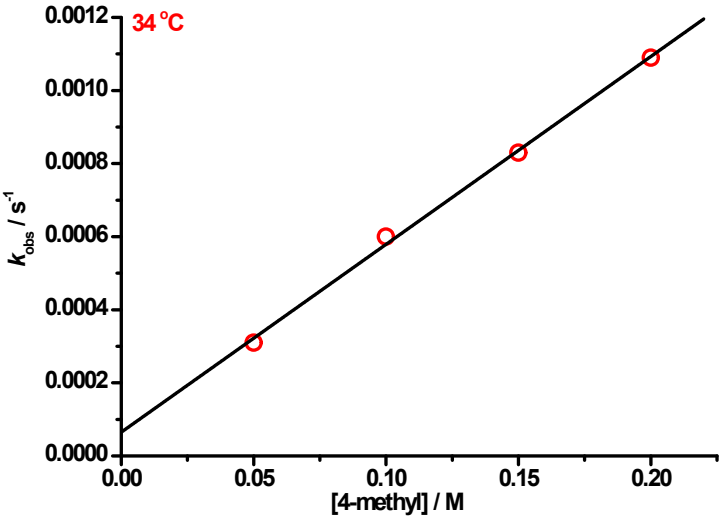


Fig. S17 Plot of k_{obs} vs [4-methyl] for the oxidation of 4-methylbenzenesulfonate by ferrate at 34 ˚C, pH=8.83 and I = 0.3 M [slope = (5.14 ± 0.16) × 10^{-3}; y-intercept = (6.50 ± 2.17) × 10^{-5}; r^2 = 0.999].

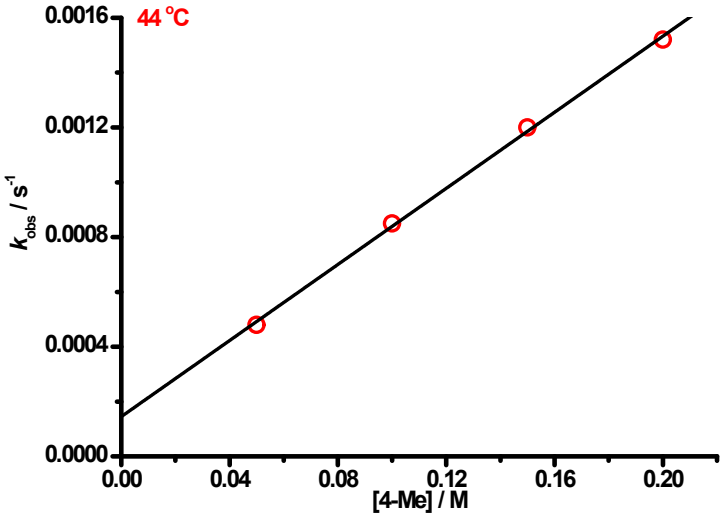


Fig. S18 Plot of k_{obs} vs [4-methyl] for the oxidation of 4-methylbenzenesulfonate by ferrate at 44 ˚C, pH=8.83 and I = 0.3 M [slope = (6.94 ± 0.16) × 10^{-3}; y-intercept = (1.45 ± 0.22) × 10^{-4}; r^2 = 0.999].

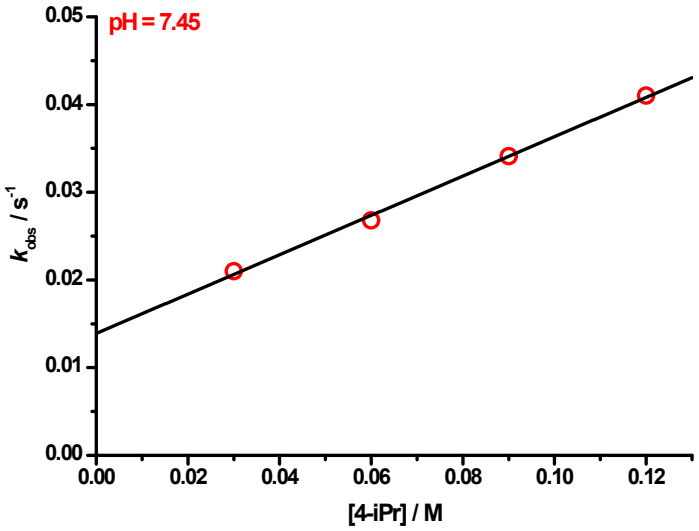


Fig. S19 Plot of k_{obs} vs [4-isopropyl] for the oxidation of 4-isopropylbenzenesulfonate by ferrate at 25 ˚C, pH=7.45 and I = 0.3 M [slope = (2.24 ± 0.07) × 10^{-1}; y-intercept =

$(1.39 \pm 0.06) \times 10^{-2}$; $r^2 = 0.999$].

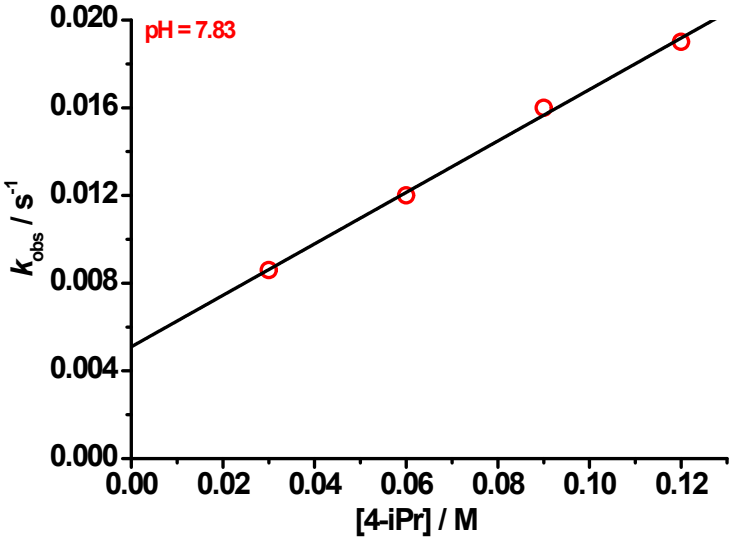


Fig. S20 Plot of k_{obs} vs [4-isopropyl] for the oxidation of 4-isopropylbenzenesulfonate by ferrate at 25 ˚C, pH=7.83 and I = 0.3 M [slope = $(1.17 \pm 0.04) \times 10^{-1}$; y-intercept = $(5.10 \pm 0.35) \times 10^{-3}$; $r^2 = 0.999$].

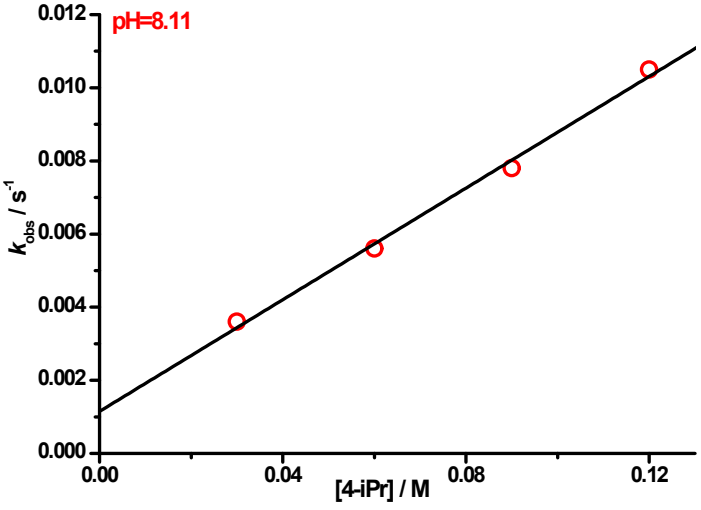


Fig. S21 Plot of k_{obs} vs [4-isopropyl] for the oxidation of 4-isopropylbenzenesulfonate by ferrate at 25 ˚C, pH=8.11 and I = 0.3 M [slope = $(7.63 \pm 0.38) \times 10^{-2}$; y-intercept =

$(1.15 \pm 0.31) \times 10^{-3}$; $r^2 = 0.998$].

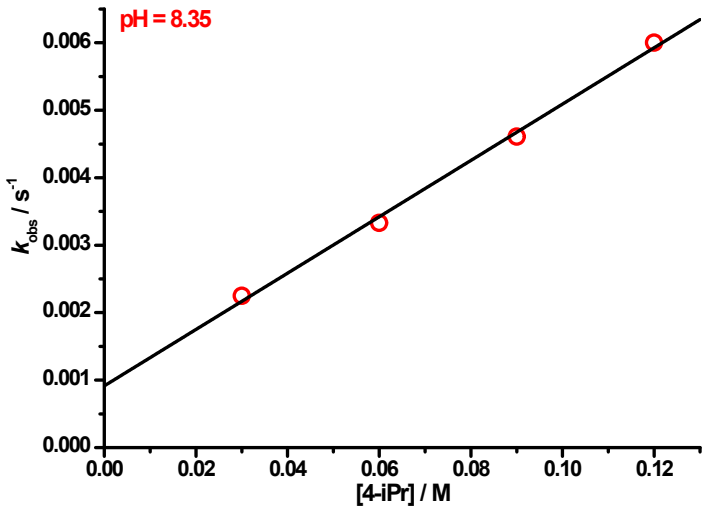


Fig. S22 Plot of k_{obs} vs [4-isopropyl] for the oxidation of 4-isopropylbenzenesulfonate by ferrate at 25 ˚C, pH=8.35 and $I = 0.3$ M [slope = $(4.18 \pm 0.17) \times 10^{-2}$; *y*-intercept = $(9.15 \pm 1.35) \times 10^{-4}$; $r^2 = 0.998$].

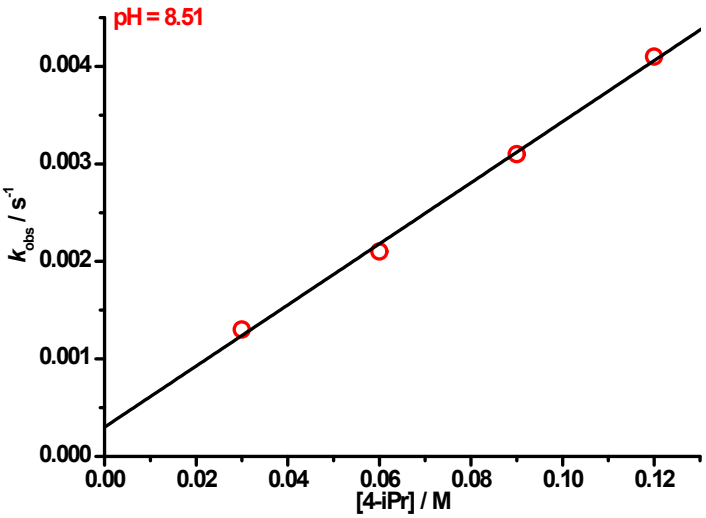


Fig. S23 Plot of k_{obs} vs [4-isopropyl] for the oxidation of 4-isopropylbenzenesulfonate by ferrate at 25 ˚C, pH=8.51 and $I = 0.3$ M [slope = $(3.13 \pm 0.12) \times 10^{-2}$; *y*-intercept =

$(3.00 \pm 0.95) \times 10^{-4}$; $r^2 = 0.999$].

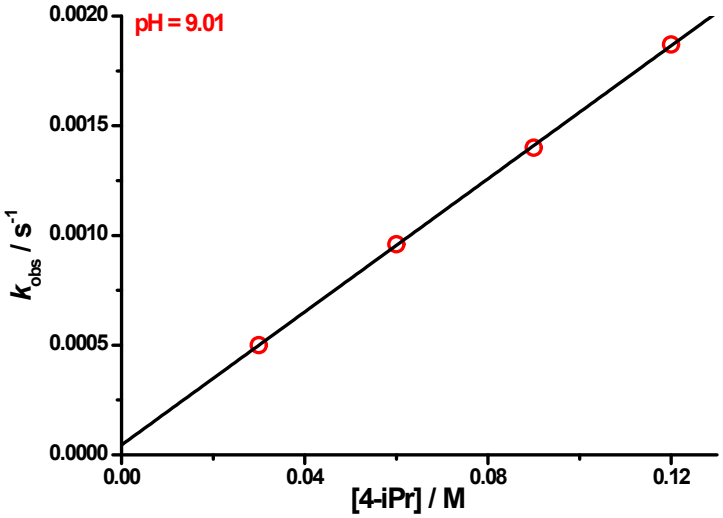


Fig. S24 Plot of k_{obs} vs [4-isopropyl] for the oxidation of 4-isopropylbenzenesulfonate by ferrate at 25 ˚C, pH=9.01 and I = 0.3 M [slope = $(1.52 \pm 0.01) \times 10^{-2}$; y-intercept = $(4.50 \pm 1.06) \times 10^{-4}$; $r^2 = 0.999$].

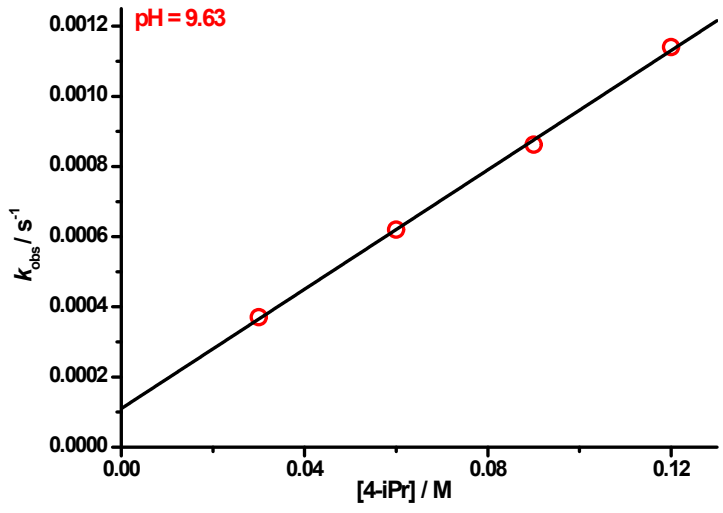


Fig. S25 Plot of k_{obs} vs [4-isopropyl] for the oxidation of 4-isopropylbenzenesulfonate by ferrate at 25 ˚C, pH=9.63 and I = 0.3 M [slope = $(8.51 \pm 0.18) \times 10^{-3}$ y-intercept =

$(1.10 \pm 0.15) \times 10^{-4}$; $r^2 = 0.999$].

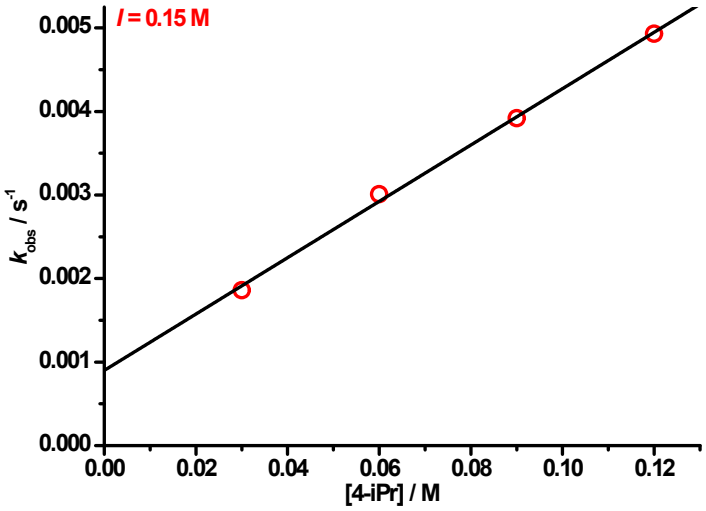


Fig. S26 Plot of k_{obs} vs [4-isopropyl] for the oxidation of 4-isopropylbenzenesulfonate by ferrate at 25 ˚C, pH=8.83 and I = 0.15 M [slope = $(3.37 \pm 0.11) \times 10^{-2}$ y-intercept = $(9.00 \pm 0.89) \times 10^{-4}$; $r^2 = 0.999$].

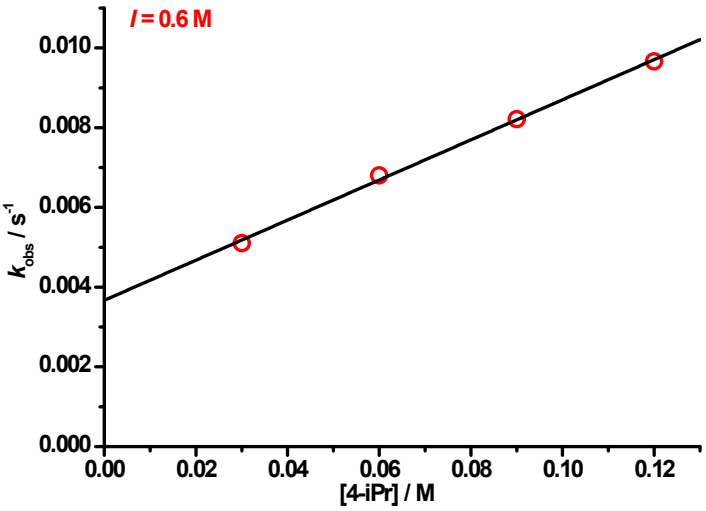


Fig. S27 Plot of k_{obs} vs [4-isopropyl] for the oxidation of 4-isopropylbenzenesulfonate

by ferrate at 25 ˚C, pH=8.83 and I = 0.6 M [slope = (5.03 ± 0.15) × 10^{-2} y-intercept = (3.17 ± 0.13) × 10^{-3}; r^2 = 0.999].

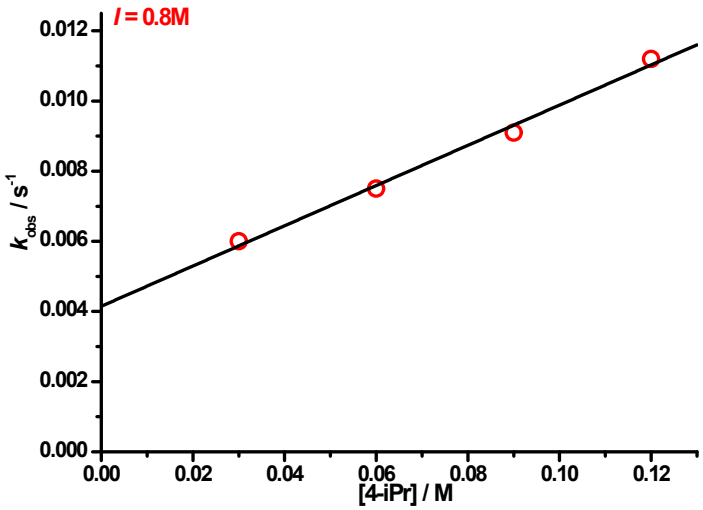


Fig. S28 Plot of k_{obs} vs [4-isopropyl] for the oxidation of 4-isopropylbenzenesulfonate by ferrate at 25 ˚C, pH=8.83 and I = 0.8 M [slope = (5.73 ± 0.33) × 10^{-2} y-intercept = (4.15 ± 0.27) × 10^{-3}; r^2 = 0.997].

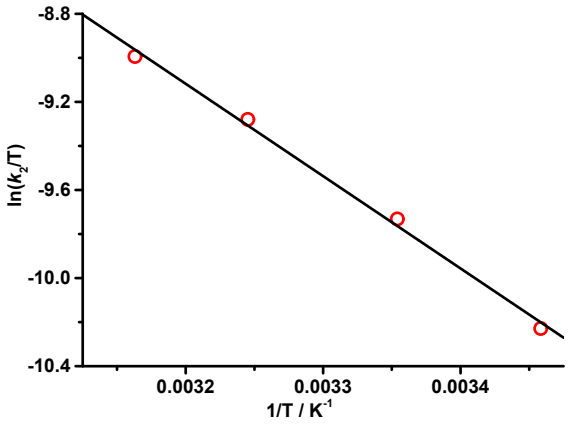


Fig. S29 Plot of k_{obs} vs [4-isopropyl] for the oxidation of 4-isopropylbenzenesulfonate by ferrate at pH=8.83 and I = 0.3 M [slope = -(4.19 ± 0.19) × 10^3; y-intercept = (4.29 ± 0.62); r^2 = 0.994].

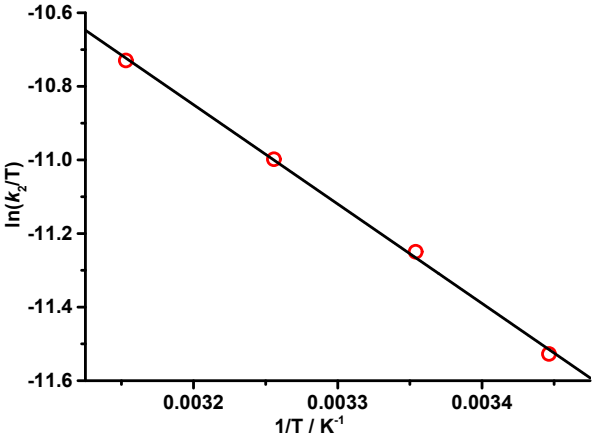


Fig. S30 Plot of k_{obs} vs [4-methyl] for the oxidation of 4-methylbenzenesulfonate by ferrate at pH=8.83 and I = 0.3 M [slope = -(2.70 ± 0.07) × 10^3; y-intercept = -(2.21 ± 0.23); r^2 = 0.998].

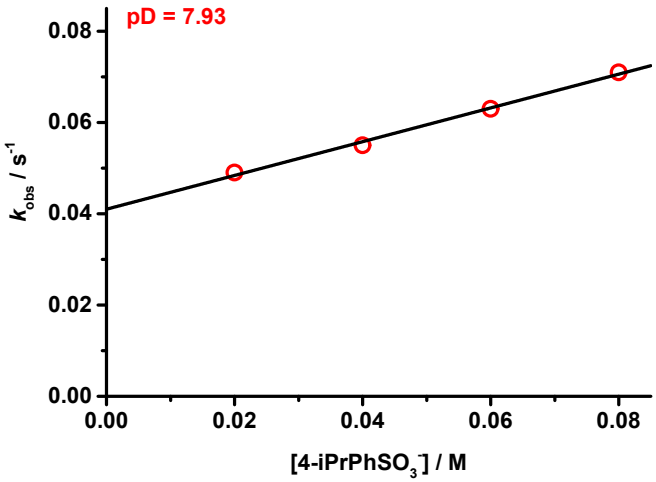


Fig. S31 Plot of k_{obs} vs [4-iPr] for the oxidation of 4-isopropylbenzenesulfonate by ferrate at 25 ˚C, pD = 7.93 and I = 0.3 M [slope = (3.70± 0.17) × 10^{-1}; y-intercept = (4.10 ±0.09) × 10^{-2}; r^2 = 0.998]

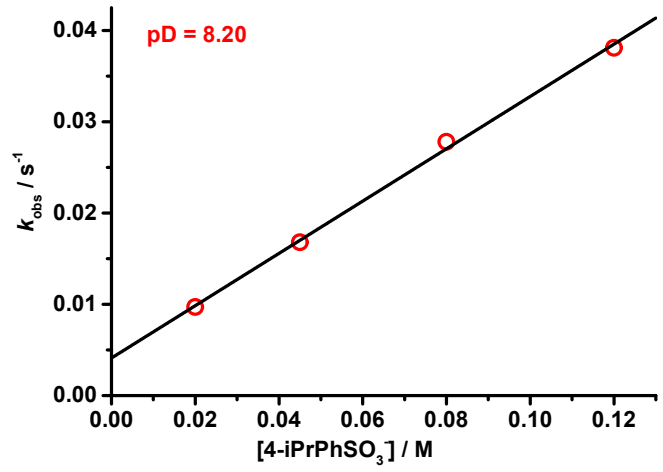


Fig. S32 Plot of k_{obs} vs [4-iPr] for the oxidation of 4-isopropylbenzenesulfonate by ferrate at 25 ˚C, pD = 8.20 and I = 0.3 M [slope = (2.87± 0.08) × 10^{-1}; y-intercept = (4.11 ±0.64) × 10^{-3}; r^2 = 0.999]

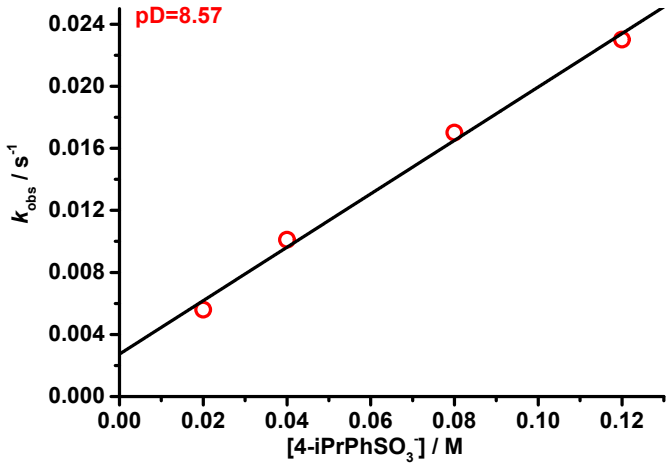


Fig. S33 Plot of k_{obs} vs [4-iPr] for the oxidation of 4-isopropylbenzenesulfonate by ferrate at 25 ˚C, pD = 8.57 and I = 0.3 M [slope = (1.72± 0.09) × 10^{-1}; y-intercept = (2.74 ±0.68) × 10^{-3}; r^2 = 0.997]

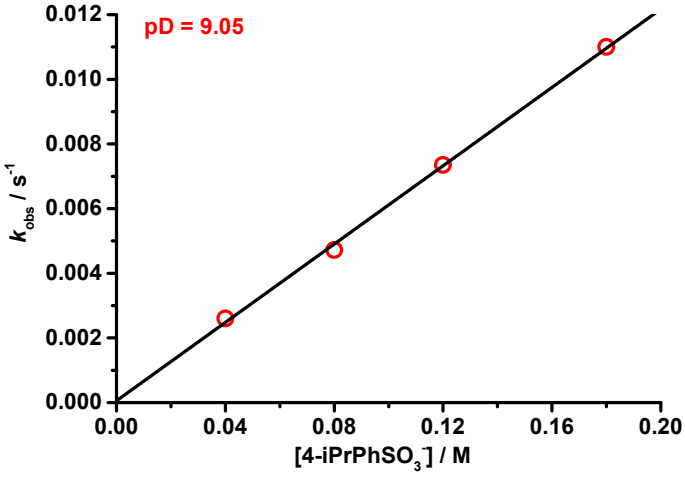


Fig. S34 Plot of k_{obs} vs [4-iPr] for the oxidation of 4-isopropylbenzenesulfonate by ferrate at 25 ˚C, pD = 9.05 and I = 0.3 M [slope = (6.06± 0.15) × 10^{-2}; y-intercept = (0.56 ± 1.79) × 10^{-4}; r^2 = 0.998]

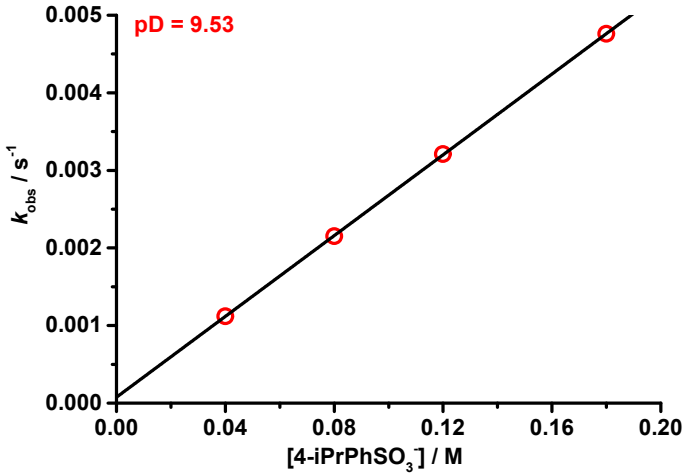


Fig. S35 Plot of k_{obs} vs [4-iPr] for the oxidation of 4-isopropylbenzenesulfonate by ferrate at 25 ˚C, pD = 9.53 and I = 0.3 M [slope = (2.60 ± 0.01) × 10^{-2}; y-intercept = (7.61 ± 1.09) × 10^{-5}; r^2 = 0.999]

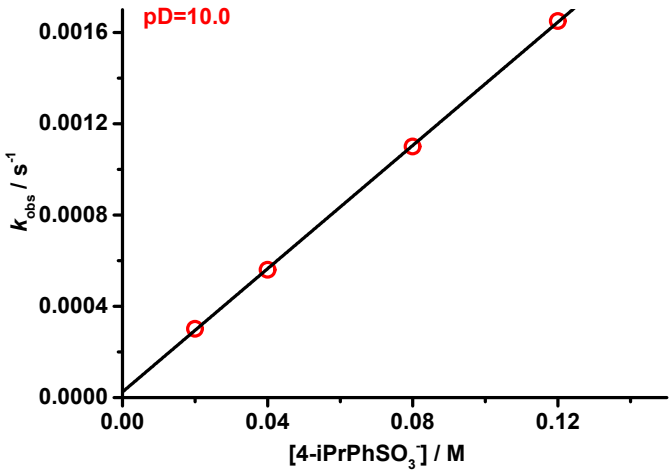


Fig. S36 Plot of k_{obs} vs [4-iPr] for the oxidation of 4-isopropylbenzenesulfonate by ferrate at 25 ˚C, pD = 10.0 and I = 0.3 M [slope = (1.35 ± 0.01) × 10^{-2}; y-intercept = (2.46 ± 0.73) × 10^{-5}; r^2 = 0.999]

Table S3 The cartesian coordinates of selected molecular species in the oxidation of isopropyl benzenesulfonate by $HFeO_4^-{\cdot}8H_2O$.

INT1

Fe	-2.4341601424	-0.2011319709	0.0585011926
O	-1.8089983783	1.2705174234	0.1189271156
O	-3.1751788353	-0.5119355964	-1.3606221258
O	-3.4036241515	-0.5179298505	1.3252973334
C	3.9212862031	1.7733464642	-0.0151488439
C	4.8974001664	0.7732621413	-0.0239312046
C	4.5112906732	-0.5689309227	0.0082220826
C	3.1547077465	-0.9078386438	0.0503045957
C	2.1893282902	0.1008038335	0.0592448537
C	2.5533643332	1.458013825	0.0259781074
H	4.2398021263	2.8165385955	-0.0404091874
H	5.9558727373	1.0274862597	-0.0538232492
H	2.8499654957	-1.9541217955	0.0771932419
H	1.1344336926	-0.176010309	0.0940098756
C	1.4882734514	2.5453435397	0.0320761685
H	0.515684024	2.03487807	0.0828562131
S	5.7539259909	-1.8856984522	-0.0192912511
O	5.4805363519	-2.7366367777	1.1876304551
O	7.0882916011	-1.2043550587	0.0355013291
O	5.5312343391	-2.6309277057	-1.3048003143
O	-5.2003421149	-2.4596678385	-1.4067085244
H	-4.4886703523	-1.7903901848	-1.4819937574
H	-5.0976954687	-3.0399081524	-2.1711729149
H	-1.3445303367	-2.2011473437	0.3777550003
O	-4.4652086603	-3.200533233	1.1725236031
H	-4.2457648299	-2.2858752891	1.4283026657
H	-4.8321133825	-3.0941925123	0.2673327168
O	-3.9117263165	3.2948491288	0.2369789164
H	-4.5463793377	2.7555031268	0.7474549786
H	-3.0862464946	2.7815013288	0.2791451361
O	-5.7816491253	1.2221266055	0.9967857969
H	-5.8204136058	1.2017755987	0.0208846072
H	-5.1176929856	0.5468043201	1.2193694804
O	-5.1469622828	1.6368252761	-1.7926961658
H	-4.6715629786	2.3694649127	-1.3559538949
H	-4.4873902495	0.9224676364	-1.837908325
O	-1.8284513044	-0.1487799298	-3.8326186813
H	-2.2386072985	-0.2475831488	-2.9518403383
H	-1.0233439615	0.3597107782	-3.6775969315
O	-2.885329835	0.7395999366	3.822032447

H	-2.3204452261	1.5057975017	3.6654636627
H	-3.0173394719	0.3381067884	2.9418979079
O	-1.0472021104	-1.2616505393	0.2006826502
C	1.5057460421	3.3693666456	-1.2673717932
H	1.3844919243	2.7236002572	-2.1481232146
H	0.6864515798	4.10283136	-1.2657237668
H	2.4500155592	3.9223690918	-1.3780544658
C	1.5970747832	3.4511299876	1.2707897052
H	1.5491297185	2.8630792588	2.1978020599
H	2.5414107082	4.0148659572	1.2741214417
H	0.773387363	4.1794896338	1.2849330982
O	-1.8544101589	-3.7847068365	0.6630876746
H	-2.8137500599	-3.7078269834	0.8970668587
H	-1.4282344454	-4.2390182083	1.4002799781

TS1

Fe	-1.8980401429	-0.0927318717	0.2739254348
O	-1.0090630592	1.3430680948	0.2430403298
O	-2.0193243472	-0.7410082706	-1.2181317524
O	-3.3127520308	0.1198549341	1.0546982911
C	3.1913311573	1.8770887699	-0.4019951196
C	4.1248608864	1.2385367334	-1.2172486666
C	4.1827802027	-0.1586081704	-1.2483666528
C	3.3029582876	-0.912926967	-0.4652173334
C	2.3756538567	-0.2661981611	0.3523580433
C	2.3044344924	1.142158561	0.411801087
H	3.1696406729	2.9650490612	-0.392625047
H	4.8064826272	1.8312985606	-1.8270295032
H	3.3466953242	-2.0002868776	-0.5024840177
H	1.6735597347	-0.8621603603	0.9339754529
C	1.2993707583	1.8092207897	1.3017104312
H	0.2153222117	1.456515245	0.8214137203
S	5.4102132399	-0.9750278232	-2.3031724386
O	5.1750291222	-0.4434273912	-3.6861689468
O	5.1475683061	-2.4445813624	-2.1836502583
O	6.7456805302	-0.5699320328	-1.7502333794
O	-4.1722474785	-2.4606456825	-1.6352116392
H	-3.3780040561	-1.8870885787	-1.5629224199
H	-3.8857502617	-3.2478049248	-2.1144217993
H	-1.243866315	-1.9128307259	1.4854425741
O	-4.5812736296	-2.4487835824	1.1285626604
H	-4.30857888	-1.5147714759	1.2185603256
H	-4.5682847928	-2.5896100499	0.1569895055
O	-2.474973886	3.3852381026	-1.065593364

H	-3.361044706	3.1095928166	-0.7636400902
H	-1.8679578438	2.8172528508	-0.5521157673
O	-4.9085631425	1.8285906565	-0.6799255318
H	-4.584056588	1.5215136637	-1.5476324563
H	-4.5032126481	1.2073522543	-0.0458969223
O	-3.165815517	1.2958682742	-2.9523414078
H	-2.7618762891	2.0862762387	-2.545197638
H	-2.7215874062	0.5518625457	-2.5044672169
O	0.3962088693	-1.1923335002	-2.613756553
H	-0.4274694849	-1.0330947529	-2.1103165644
H	1.1070737395	-0.9501567085	-2.0057846082
O	-3.2054449279	2.1080580014	3.0544724891
H	-2.4552891631	2.6670194561	2.8190856367
H	-3.223472735	1.4131962782	2.3652629847
O	-0.8117401955	-1.0462435674	1.2772714833
C	1.2235348835	3.3267720954	1.2212507753
H	1.0889010965	3.6821729919	0.1919705357
H	0.3811664877	3.6941664786	1.8201124155
H	2.140083889	3.7867359223	1.62460745
C	1.2567008351	1.2969445846	2.739823146
H	1.2428051174	0.2041544193	2.7980865851
H	2.1437264551	1.6613214805	3.2836531013
H	0.3657032302	1.6778075637	3.2563906607
O	-2.1215052869	-3.41546731	1.8550861124
H	-3.0601356683	-3.1717921933	1.66079748
H	-2.1034965715	-3.7034450442	2.7757872623

INT2

Fe	2.1607068056	-0.3968283178	-0.0540425093
O	1.3389011275	1.1285507629	-0.472120428
O	2.5553147238	-0.4130556514	1.515488567
O	3.3016489972	-0.7156521516	-1.1557275611
C	-2.2048241462	1.6930811315	1.0294830515
C	-2.8557375561	0.5632407053	1.5120232974
C	-3.3328473875	-0.4097317341	0.6225673189
C	-3.1588221091	-0.2351235771	-0.7605792111
C	-2.5166892736	0.8942560131	-1.2456699351
C	-2.0101525325	1.9066293439	-0.3702214967
H	-1.8512024042	2.4337680847	1.7442719309
H	-3.008613374	0.4283597043	2.5822182736
H	-3.5299397071	-0.9871519689	-1.4569710614
H	-2.4005211777	1.0035292401	-2.3224876989
C	-1.3506036058	3.0728158785	-0.8709191307
H	0.4004152513	0.9429220877	-0.6354422409

S	-4.1835288272	-1.8815346139	1.2321582588
O	-5.563512641	-1.8301095228	0.6403683487
O	-4.184028976	-1.7733663147	2.7270020423
O	-3.3912949474	-3.0535159766	0.7280512499
O	3.4117207537	-3.0826239518	2.1348175891
H	3.1657169214	-2.1412022098	2.0443284305
H	2.5991787698	-3.5579790872	1.9004414485
H	0.8910236408	-2.2908332069	-0.2017902659
O	4.1050832357	-3.4552860355	-0.6137714002
H	3.9681765736	-2.5465524313	-0.9412179176
H	4.1562968231	-3.343468292	0.3571362552
O	3.138916197	3.2469246318	-0.3333673536
H	3.8942594835	2.7920506054	-0.7483771569
H	2.3968532808	2.6186974981	-0.4466228281
O	5.3511106023	1.3549770256	-0.7235030938
H	5.2558421577	1.4273249452	0.2458706009
H	4.7864863139	0.5951883028	-0.9536950555
O	4.3029222794	1.8838982869	1.9253243396
H	3.8104690863	2.5156773672	1.3647632444
H	3.7269490797	1.0973297735	1.9484499454
O	0.2391758425	-0.2977422511	3.1858222801
H	1.0302315932	-0.347985898	2.6147725976
H	-0.4968923865	-0.1719008798	2.5730834954
O	2.703789965	0.4663175286	-3.6661281235
H	2.0558165896	1.1480110204	-3.4506374232
H	2.8963928507	0.0361440075	-2.8097551244
O	0.6979334859	-1.3358067608	-0.3447269996
C	-0.8231896409	4.1136067265	0.0741675001
H	-0.1503290321	3.6797092066	0.8305599331
H	-0.2701410902	4.8936932954	-0.4602086573
H	-1.6394889122	4.6063888294	0.6318784689
C	-1.220178646	3.2991385215	-2.3502364265
H	-0.6504697768	2.4941127423	-2.844287897
H	-2.205421841	3.3263194931	-2.8466408464
H	-0.7120212296	4.2453660454	-2.5645018905
O	1.4735395895	-4.016801268	0.0345669608
H	2.3604220408	-4.002921182	-0.3914229904
H	0.9764601595	-4.7382605223	-0.3693307047

TS2

Fe	-2.08075300	-0.40673100	-0.29546500
O	-0.80666300	0.85247500	-0.48924600
O	-3.52647100	0.07707900	-0.88660700
O	-2.03557700	-1.06614900	1.19863000

C	2.86683500	1.17238500	-1.60092700
C	3.90679500	0.27910300	-1.36947400
C	4.32508300	0.01200300	-0.06070300
C	3.69018200	0.65031500	1.01848100
C	2.65176300	1.53963800	0.78873400
C	2.19501700	1.83917900	-0.53313400
H	2.57313500	1.36200300	-2.63111200
H	4.40285400	-0.21598000	-2.20252400
H	4.01098400	0.44675700	2.03988200
H	2.18240100	2.01287300	1.64799100
H	-0.15014100	0.45610300	-1.08296100
S	5.69298700	-1.12535700	0.25973700
O	6.79641100	-0.27803100	0.82600400
O	6.04540600	-1.73609600	-1.06207700
O	5.17145500	-2.12310300	1.25215500
O	-5.62576100	-1.63361100	-0.28769900
H	-4.92473700	-1.00707300	-0.57121400
H	-6.01303300	-1.97986100	-1.10306200
H	-1.70902600	-2.35425800	-1.47270200
O	-3.77745700	-3.32512100	0.97574700
H	-3.14258600	-2.61938500	1.20989300
H	-4.55205000	-2.83190500	0.62745300
O	-2.89513000	3.01955400	2.71747600
H	-2.98247300	2.07661100	2.97394800
H	-1.94822500	3.16608300	2.61117300
O	-3.70310000	0.36133700	2.98427700
H	-4.36261800	0.68918800	2.34457000
H	-3.09985000	-0.18002500	2.43141900
O	-4.89577900	1.93244900	0.78642000
H	-4.23745300	2.53106300	1.18223600
H	-4.39741900	1.38927200	0.14363600
O	-3.98511400	0.82546100	-3.52089800
H	-3.77026200	0.58373600	-2.59437000
H	-3.53764300	1.66807500	-3.66911300
O	0.51807800	-1.13754800	2.35933400
H	1.07228700	-0.55105400	1.82908700
H	-0.36230300	-1.10896300	1.92947900
O	-1.26124900	-1.47771700	-1.44450100
O	-2.52536500	-3.98705300	-1.37180600
H	-2.99281700	-3.87996400	-0.50769600
H	-1.91978000	-4.72948700	-1.25623300
C	1.12625400	2.76281100	-0.78323000
C	0.70335200	3.10454700	-2.18145800
H	-0.30619500	3.53323800	-2.18607200

H	1.38067200	3.86805500	-2.60661200
H	0.71635200	2.24890300	-2.86683100
C	0.53650500	3.62904800	0.28349600
H	0.88359800	4.67053900	0.15323800
H	-0.55790500	3.65422000	0.18699100
H	0.79584100	3.31637700	1.29741700

INT3

Fe	-2.2686647359	0.309811044	0.5413413196
O	-0.2683317452	-0.3207864956	1.0305103133
O	-3.3296447156	-0.9576474019	0.7091888665
O	-2.5386202564	1.2775546048	-0.7837130131
C	3.2019493251	-1.4348233288	0.9618902574
C	4.4655963753	-0.8736733828	0.7441730423
C	4.576220121	0.3379009108	0.0639215243
C	3.4275788603	0.9893121524	-0.4035122177
C	2.1742150806	0.4221720597	-0.1850492151
C	2.0420994855	-0.7991174068	0.5023343664
H	3.1394361476	-2.3805063725	1.4971831823
H	5.3628690842	-1.3732583452	1.1054217969
H	3.5104045946	1.9368392646	-0.9357261412
H	1.2875659964	0.9398900154	-0.5495185897
H	-0.0317519356	0.1002770306	1.8694713932
S	6.2004599233	1.0917000956	-0.2183987567
O	6.3349494071	1.2209768526	-1.7079190496
O	7.2045062552	0.1557199733	0.3822509844
O	6.1539413558	2.4244320321	0.4712532443
O	-5.9248032642	-0.1376389557	0.5008246982
H	-5.0053226009	-0.4832957847	0.6328748305
H	-6.3708562803	-0.2423872411	1.3497419231
H	-2.8150852485	1.8863846647	2.194054121
O	-5.0169377452	2.4229861684	-0.2028061491
H	-4.1332096331	2.1106910147	-0.5062204622
H	-5.4890317541	1.5870117828	0.0023738389
O	-2.1156902077	-2.1701178308	-3.6522679989
H	-2.5033818963	-1.2736142712	-3.5426497264
H	-1.1593307243	-2.0556076338	-3.6028461071
O	-3.6953006739	0.0014495096	-2.9464045101
H	-4.1642062348	-0.7230387727	-2.4930905876
H	-3.2717969899	0.4961650995	-2.2056082186
O	-4.0512702094	-2.5060529103	-1.5065229482
H	-3.272773268	-2.6537337244	-2.0718053565
H	-3.7199011902	-2.0244864064	-0.717134556
O	-3.066679534	-2.8841710664	2.6511877199

H	-3.144974057	-2.1736888386	1.9726961709
H	-3.9667775746	-3.0348851751	2.9601369774
O	-0.3449512747	2.5573736433	-1.8502746591
H	-0.6996666299	3.2732549607	-2.3889836515
H	-1.13299698	2.111808827	-1.4610280969
O	-2.0530143259	1.2970068655	2.0120445215
O	-4.2626641503	3.0506113812	2.3438568302
H	-4.5948343258	2.9371666081	1.4179586974
H	-4.0272398662	3.9822687689	2.4288904602
C	0.6463712015	-1.4044007729	0.6933014918
C	0.5700177557	-2.4482348898	1.8094564181
H	-0.4775156138	-2.7274306837	1.9694419705
H	1.1293902831	-3.3539759749	1.5443091166
H	0.9757290696	-2.0550687494	2.7513125936
C	0.1314161559	-1.979548673	-0.6295820071
H	0.7980864694	-2.7801774911	-0.970895957
H	-0.8765155037	-2.3924931545	-0.4981432075
H	0.099851378	-1.200032456	-1.400636788