Electronic Supplementary Information

Relative and inherent reactivity of imidazolium-based ionic liquids: the implications for lignocellulose processing

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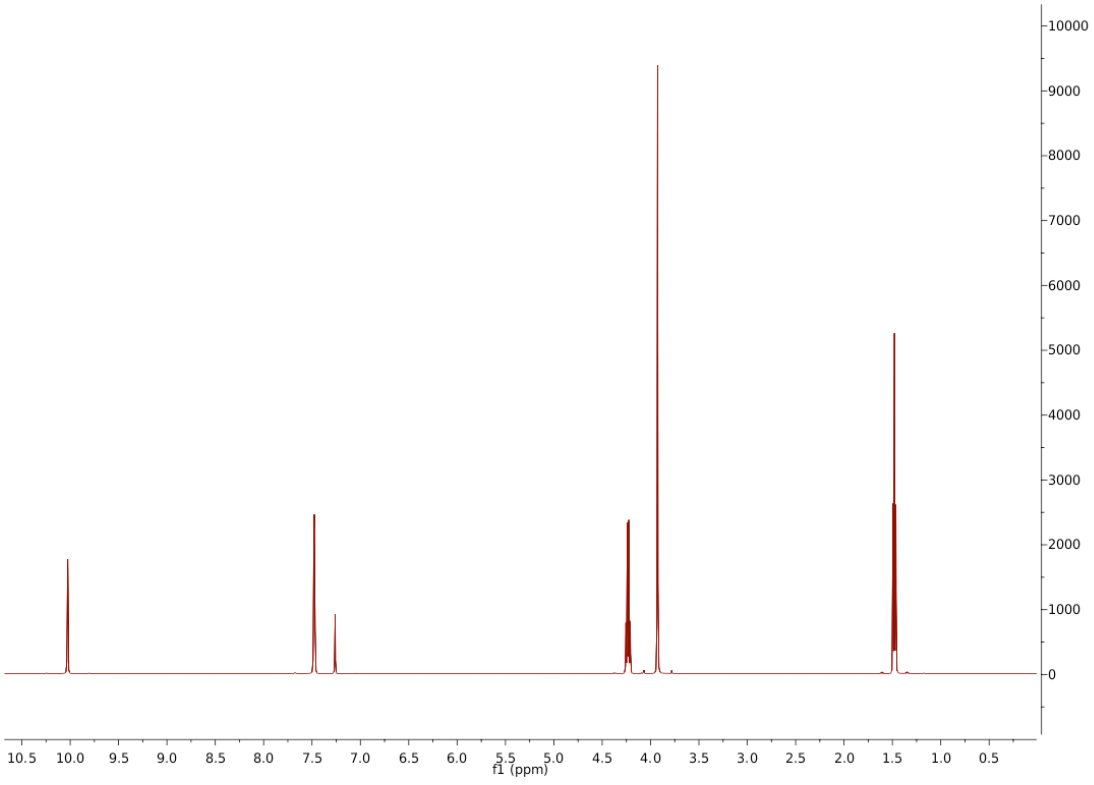
S1. Materials

1-Ethyl-3-methylimidazolium acetate ([emim][OAc], >95 %), 1-ethyl-3-methylimidazolium nitrate ([emim][NO_3], >98 %), 1-ethyl-3-methylimidazolium bromide ([emim]Br, 99 %), 1-ethyl-3-methylimidazolium iodide ([emim]I, >98 %), 1-ethyl-3-methylimidazolium tosylate ([emim][OTs], 99 %), 1-ethyl-3-methylimidazolium trifluoroacetate ([emim][CF_3CO_2], >97 %) were purchased from IoLiTec GmbH and used without further purification. 1-ethyl-3-methylimidazolium ethylsulphate ([emim][$EtSO_4$], 99 %), 1-ethyl-3-methylimidazolium bis(trifluoromethylsulphonyl)imide ([emim][NTf_2], 99 %) and [emim][NTf_2] (Solvent Innovation (Merck), 99 %) were provided by Solvent Innovation GmbH (now Merck KGaA) and were used without further purification. 1-ethyl-3-methylimidazolium chloride ([emim]Cl, 'for synthesis'), 1-ethyl-3-methylimidazolium thiocyanate ([emim][NCS], 'for synthesis'), 1-ethyl-3-methylimidazolium tris(pentafluoroethyl)trifluorophosphate ([emim][FAP], 'high purity') were provided by Merck KGaA and used without further purification. Dimethylphosphite, methyl methanesulphonate, methyl trifluoromethanesulphonate, silver acetate and trimethylphosphate were purchased from Aldrich and used without further purification.

S2. Synthesis of [emim][NO_2]

$AgNO_2$ (9.35 g, 0.0608 mol) was added to [emim]Cl (10 g, 0.0608 mol) in distilled water (50 mL) and the solution was allowed to stir for 18 h at room temperature. The solution was filtered through celite and allowed to stand in a refrigerator for 18 h. The mixture was filtered again due to precipitation of further salt and evaporated at 95 ^{o}C. Most of the solvent was removed by rotary evaporation at 60 ^{o}C, followed by rotary evaporation under high vacuum for 2 h, to yield a white crystalline solid (10.12 g, 96%). m.p. 65-70 ^{o}C (lit[1] 55 ^{o}C, MeCN/Et_2O); ^{1}H NMR (500 MHz, $CDCl_3$): δ 1.48 (3H, t, *J*=7.4 Hz), 3.93 (3H, s), 4.23 (2H, q, *J*=7.4 Hz), 7.48 (2H, m), 10.03 (1H, s); ^{13}C NMR (125 MHz, $CDCl_3$): δ 15.67, 36.47, 45.27, 122.21, 123.88, 137.81; IR (ATR, cm^{-1}) 3153 (CH_3), 3061 (CH_2), 3022 (CH_3), 2877 (CH_2) 1571 (C=N, C=C), 1211 (NO_2), 896 (NO_2).

^{1}H NMR Spectra:

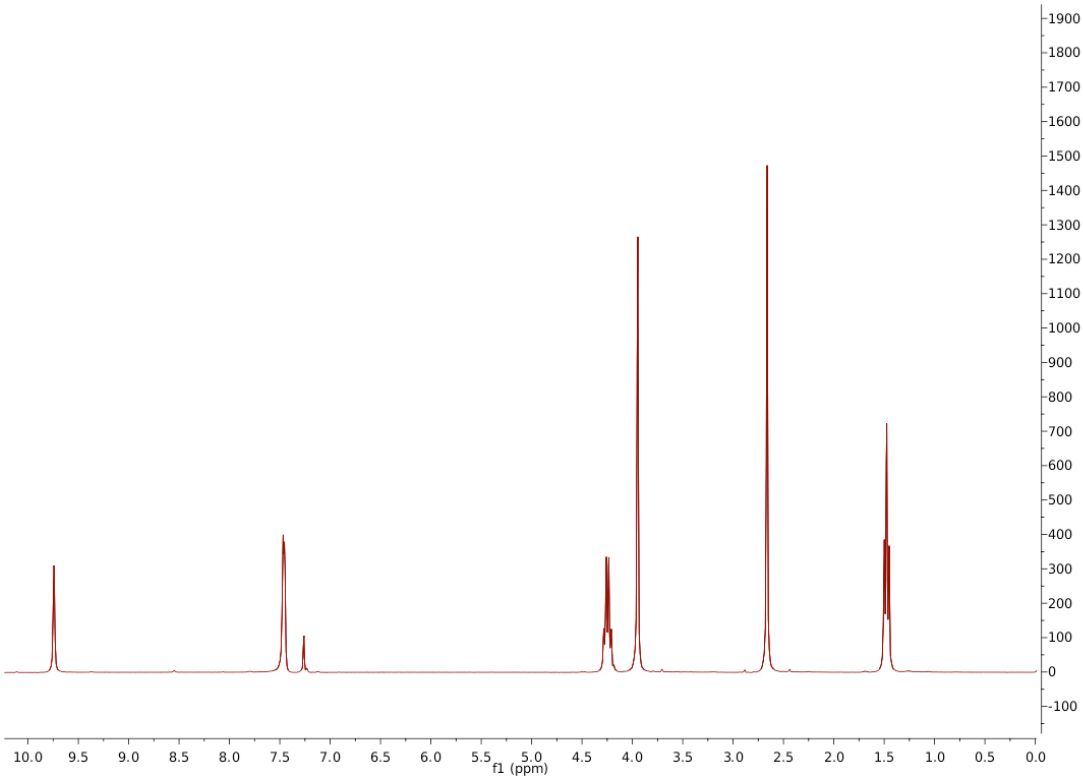


1 J. S. Wilkes and M. J. Zaworotko, Air and water stable 1-ethyl-3-methylimidazolium based ionic liquids, *J. Chem. Soc., Chem. Commun*. 1992, **13**, 965-967.

S3. Synthesis of [emim][OMs]

1-Ethylimidazole (8.73 g, 0.0908 mol) was added dropwise (over 30 min) to neat methyl methanesulphonate (10 g, 0.0908 mol) at room temperature. The reaction was exothermic and the solution was allowed to stir for a further 18 h at room temperature. The mixture was rotary evaporated at 65 ^{o}C under high vacuum for 18 h, to yield a clear pale grey oil (18.70 g, 100%). ^{1}H NMR (300 MHz, $CDCl_3$): δ 1.48 (3H, t, *J*=7.3 Hz), 2.66 (3H, s), 3.95 (3H, s), 4.23 (2H, q, *J*=7.4 Hz), 7.46 (2H, m), 9.74 (1H, s); IR (ATR, cm^{-1}) 3146 (CH_3), 3088 (CH_2), 1571 (C=N, C=C), 1178 (CH_3), 1460 (CH_3), 1028 (SO_3).

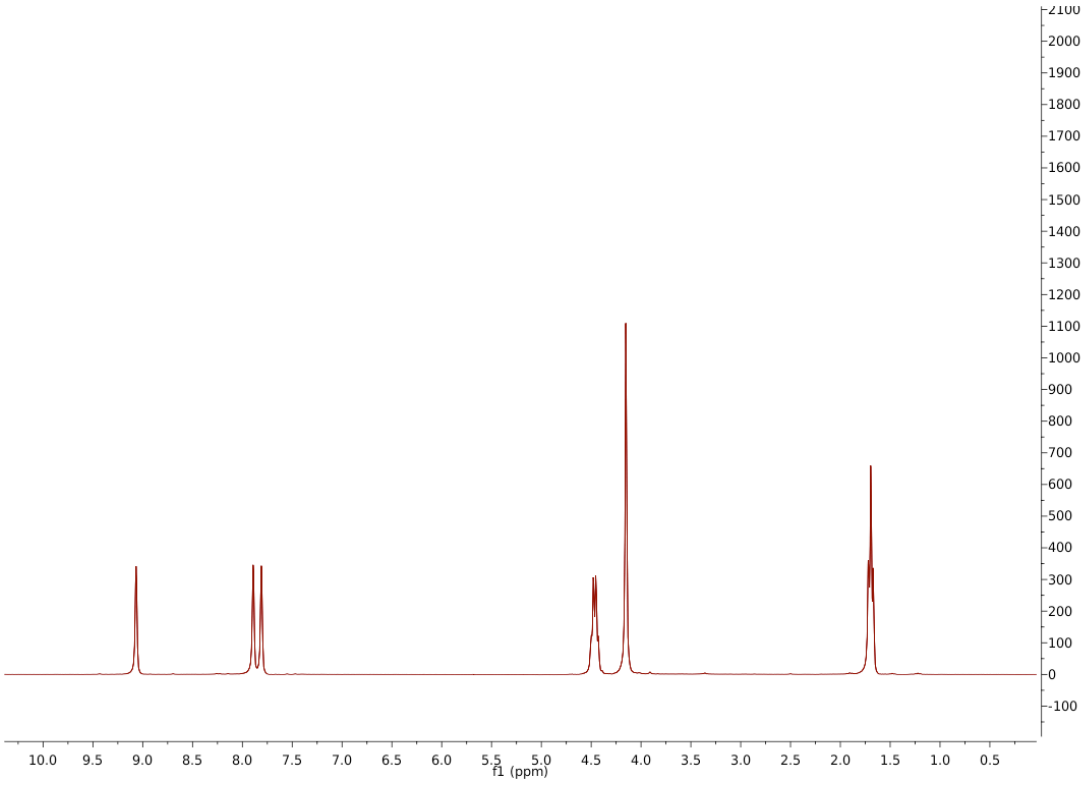
^{1}H NMR Spectra:



S4. Synthesis of [emim][OTf]

1-Ethylimidazole (5.86 g, 0.0609 mol) was added dropwise (over 1 h) to neat methyl trifluoromethylsulphonate (10 g, 0.0609 mol) in an ice bath. The reaction was very exothermic and the solution was allowed to stir for a further 18 h at room temperature. The mixture was rotary evaporated at 65 ^{o}C under high vacuum for 18 h, to yield a clear pale yellow oil (15.80 g, 100%). ^{1}H NMR (300 MHz, neat with DMSO-d6 capillary insert): δ 1.92 (3H, t, *J*=7.2 Hz), 4.37 (3H, s), 4.65-4.88 (2H, q, *J*=7.3 Hz), 8.03 (1H, s), 8.11 (1H, s), 9.29 (1H, s); IR (ATR, cm^{-1}) 3159 (CH_3), 3120 (CH_2), 2982 (CH_3), 1578 (C=N, C=C), 1454 (CH_3), 1251 (CF_3), 1145 (CF_3), 640 (CF_3).

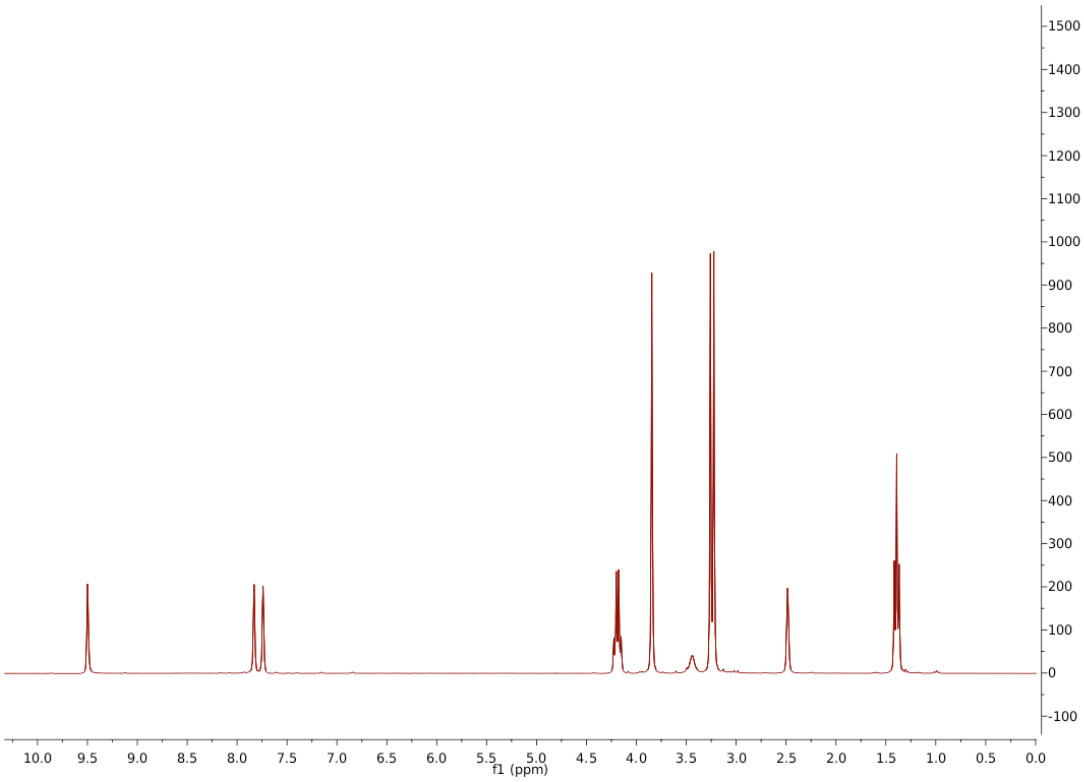
^{1}H NMR Spectra:



S5. Synthesis of [emim][Me_2PO_4]

1-Ethylimidazole (48.0 g, 0.500 mol) was added dropwise (over 1 h) to neat trimethylphosphate (70.0 g, 0.500 mol) at 100 ^{o}C. The reaction was allowed to stir for a further 18 h at 80 ^{o}C. The mixture was rotary evaporated at 65 ^{o}C under high vacuum for 18 h, to yield a clear pale yellow oil (118.0 g, 100%). ^{1}H NMR (300 MHz, DMSO-d6): δ 1.39 (3H, t, *J*=7.3 Hz), 3.24 (6H, d, *J*=10.3 Hz), 3.85 (3H, s), 4.19 (2H, q, *J*=7.3 Hz), 7.74 (1H, s), 7.83 (1H, s), 9.50 (1H, s); IR (ATR, cm^{-1}) 3139 (CH_3), 3055 (CH_2), 2936 (CH_3), 1565 (C=N, C=C), 1460 (CH_3), 1231 (CH_3), 1034 (Me_2PO_4), 765 (Me_2PO_4).

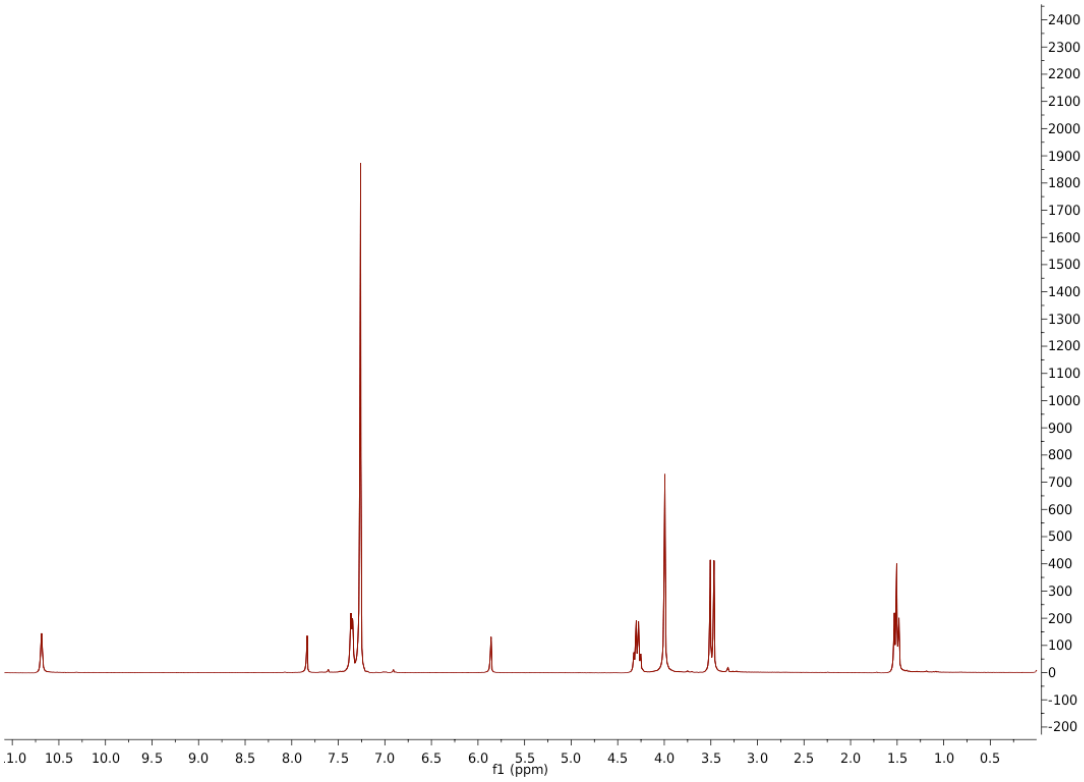
^{1}H NMR Spectra:



S6. Synthesis of [emim][MeHPO$_3$]

1-Ethylimidazole (96.1 g, 1.00 mol) was added dropwise (over 1 h) to neat dimethylphosphite (110.0 g, 1.00 mol) at 85 ^{o}C. The reaction was allowed to stir for a further 18 h at 80 ^{o}C. The mixture was rotary evaporated at 65 ^{o}C under high vacuum for 18 h, to yield a clear pale yellow oil (206.0 g, 100%). ^{1}H NMR (300 MHz, $CDCl_3$): δ 1.50 (3H, t, *J*=7.3 Hz), 3.49 (3H, d, *J*=11.8 Hz), 4.00 (3H, s), 4.29 (2H, q, *J*=7.3 Hz), 6.85 (1H, d, *J*=594 Hz), 7.36 (2H, m), 10.69 (1H, s); IR (ATR, cm^{-1}) 3146 (CH_3), 3048 (CH_2), 2943 (CH_3), 2300 (PH), 1571 (C=N, C=C), 1460 (CH_3), 1231 (CH_3), 1178 ($MeHPO_3$), 1047 ($MeHPO_3$).

^{1}H NMR Spectra:



S7. *Distillation of [emim][OAc]*.

Distillation vacuum was achieved using an oil pulp connected to a Pfeiffer TPH 330 turbo pump. Pressure at the turbo pump head was typically < 0.0008 mbar. Pressure at the sublimation apparatus was as low as 0.02 mbar prior to distillation. Pressure at the Büchi Kugelrohr was 0.2 mbar, prior to distillation.

S8. Chloride determination for [emim][NO_2]

Ion chromatography was performed using a Dionex ICS-1500 ion chromatography system, with an Ionpack(R) AS9-HC analytical column. Samples (6.68 and 19.82 mg) were diluted with 100 ml water. Detection of peaks was by conductivity demonstrating a single peak.

Argentometric titration of chloride was done with a Mettler-Toledo DL53+ automatic titrator, using the manufacturer's program for argentometry. The electrode was DM 141-SC and the titrant 0.1 M $AgNO_3$, added in >0.02 ml increments. 20-70 mg sample was mixed with 30 ml of water, 2 drops of 10% HNO_3 was added and the sample titrated. Verification was performed with NaCl and [emim]Cl and the chloride content of [emim][NO_2] determined to be negligible.

S9. Thermogravimetric Analysis.

TGAs were determined using a Mettler Toledo TGA/SDA 851e, using a standard temperature program with 10 $^{o}C\ min^{-1}$ heating rate from 50-600 ^{o}C on 10-15 mg of sample. The temperatures, at which the maximum rate of decomposition was observed, for correlation with proton affinities, were obtained by taking the 1st derivatives of the TGA traces. The temperature at which the 1st derivative trace reached its lowest point was taken to be the maximum rate of decomposition.

S10. Proton Affinity Calculations.

Protonated and unprotonated structures were created and minimised at the MMFF94 level using Avogadro (http://sourceforge.net/projects/avogadro/). The geometries were further minimized at the RHF/STO-3G level in GAMESS 2009, compiled for 64-bit Ubuntu. Concurrent optimization and vibrational frequency calculations were performed at the MP2/6-311+G(d,p) level. A typical input file is as follows:

```
 $CONTRL SCFTYP=RHF MPLEVL=2 RUNTYP=OPTIMIZE QMTTOL=0.0000001 ICUT=11
  ICHARG=-1 MULT=1 COORD=UNIQUE $END
 $SYSTEM MEMORY=400000000 $END
 $BASIS GBASIS=N311 NGAUSS=6 NDFUNC=1 NPFUNC=1 DIFFSP=.TRUE. $END
 $STATPT NSTEP=500 OPTTOL=0.00001 HSSEND=.T. $END
 $FORCE  PURIFY=.T. NVIB=2 $END
 $ZMAT DLC=.T. AUTO=.T. $END
 $SCF DIRSCF=.T. DIIS=.T. FDIFF=.F. $END
 $DATA
Cl Anion MP2 6-311+G(d,p) Hessian
C1
Cl 17 0.00000000 0.00000000 0.00000000
 $END
```

Structures were reoptimised if imaginary frequencies were observed in the output. Imaginary frequencies for all but one structure were eliminated (see Tetracyanoborate optimised geometry below). This imaginary frequency was not included in the thermochemical calculation. The proton affinity values were calculated as follows:

for the following reactions (- DH_{PA}):

$X^- + H^+ \longrightarrow [XH]$ **or** $X: + H^+ \longrightarrow [XH]^+$

$-DH_{PA} = E_H + E_X - E_{XH} + RT$

E_H = 3/2RT (translational energy of a proton – proton does not contain rotational, vibrational or electronic energies)

$E_{X/XH} = E_{elec} + E_{rot} + E_{trans} + ZPE$

E_{elec} (electronic energy) & ZPE (zero-point energy) are obtained from the GAMESS outputs.

E_{rot} = RT (rotational energy for linear species)

E_{rot} = 3/2RT (rotational energy for non-linear polyatomic species)

E_{trans} = 3/2RT (translational energy for all species)

R = 0.0019872 kcal mol^{-1} K^{-1}

T = 298.15 K

Proton affinity values were rapidly processed using a python script:

```
#####################################################################START
#Python script for determining proton affinities from 2 GAMESS output files by Alistair W. T. King

import sys

#check for arguements
if len(sys.argv) != 5:
        print 'Usage: python protonaffinity.py <acidfile.out> <basefile.out> <Acid Geometry> <Base Geometry>\n'
        print 'Acid & Base Geometries M (Monoatomic), L (Linear), N (Non-linear)\n'
        print len(sys.argv)
        sys.exit(1)
Acidfilename=sys.argv[1]
Basefilename=sys.argv[2]
AcidGeom=str(sys.argv[3])
BaseGeom=str(sys.argv[4])
```

```
#some constants
H2kcal = 627.53 # for conversion from Hartrees to kcals
T = 298.15 # Kelvin
R = 0.0019872 # kcal.mol-1.K-1

##################acid energy#####################
#open the file, copy as a string and close
Acidfile=open(Acidfilename)
Afilestring=Acidfile.read()
Acidfile.close()
#rfind to locate the last ENERGY COMPONENTS in the string
index = Afilestring.rfind('ENERGY COMPONENTS', 1)
index = Afilestring.find('TOTAL ENERGY', index)
AElec = H2kcal*float(Afilestring[index+14:index+35])
print "\nThe electronic energy for the protonated species is " + str(AElec) + " kcal/mol"
#locate the THERMOCHEMISTRY section in the string
index = Afilestring.rfind('THE HARMONIC ZERO POINT ENERGY IS', 1)
if index == -1:
        AHZPE = 0
else:
        index = Afilestring.find('CM**-1/MOLECULE', index)
        AHZPE = float(Afilestring[index+20:index+33])
print "The harmonic zero-point energy for the protonated species is " + str(AHZPE) + "
kcal/mol\n"
#determine weather monoatomic, diatomic or non-linear
if AcidGeom == 'M':
        AErot = 0
        AEtrans = R*T*3/2
        print "Note: The Acid is assumed to be monoatomic!"
elif AcidGeom == 'N':
        AErot = R*T*3/2
        AEtrans = R*T*3/2
        print "Note: The Acid is assumed to be non-linear!"
elif AcidGeom == 'L':
        AErot = R*T
        AEtrans = R*T*3/2
        print "Note: The Acid is assumed to be linear!"
else:
   print "Please Check the input parameters for the Acid Geometry\n"

##################base energy#####################
#open the file, copy as a string and close
Basefile=open(Basefilename)
Bfilestring=Basefile.read()
Basefile.close()
#rfind to locate the last ENERGY COMPONENTS in the string
index = Bfilestring.rfind('ENERGY COMPONENTS', 1)
index = Bfilestring.find('TOTAL ENERGY', index)
BElec = H2kcal*float(Bfilestring[index+14:index+35])
print "\nThe electronic energy for the unprotonated species is " + str(BElec) + " kcal/mol"
#locate the THERMOCHEMISTRY section in the string
index = Bfilestring.rfind('THE HARMONIC ZERO POINT', 1)
if index == -1:
        BHZPE = 0
else:
```

```
        index = Bfilestring.find('CM**-1/MOLECULE', index)
        BHZPE = float(Bfilestring[index+20:index+33])
print "The harmonic zero-point energy for the unprotonated species is " + str(BHZPE) + "
kcal/mol\n"
#determine weather monoatomic, diatomic or non-linear
if BaseGeom == 'M':
        BErot = 0
        BEtrans = R*T*3/2
        print "Note: The Base is assumed to be monoatomic!"
elif BaseGeom == 'N':
        BErot = R*T*3/2
        BEtrans = R*T*3/2
        print "Note: The Base is assumed to be non-linear!"
elif BaseGeom == 'L':
        BErot = R*T
        BEtrans = R*T*3/2
        print "Note: The Base is assumed to be linear!"
else:
   print "Please Check the input parameters for the Base Geometry\n"

################final calculation################
AE = AErot+AEtrans+AElec+AHZPE
print "The acid total energy is " + str(AE) + " kcal/mol\n"
BE = BErot+BEtrans+BElec+BHZPE
print "The base total energy is " + str(BE) + " kcal/mol\n"
deltaE = AE - BE
PA =  R*T*5/2 - deltaE
PA*=-1
print "The proton affinity is " + str(PA) + " kcal/mol\n\n"
#####################################################HAPPY ENDING
```

S11. Van der Waals Surface Area and Volume Calculations.

The MP2/6-311+G(d,p) optimised geometries for the ionic liquid anions were submitted for a 'polarisable continuum model' **REF** solvation energy calculation, with the van der Waals radii scaled by a value of 1 (ALPHA=1), corresponding to the van der Waals cavity. Both the van der Waals surface area and volume were taken from the output files. A typical input file was as follows:

```
 $CONTRL SCFTYP=RHF MPLEVL=2 RUNTYP=ENERGY QMTTOL=0.0000001 ICUT=11
  ICHARG=-1 MULT=1 COORD=UNIQUE $END
 $SYSTEM MEMORY=400000000 $END
 $BASIS GBASIS=N311 NGAUSS=6 NDFUNC=1 NPFUNC=1 DIFFSP=.TRUE. $END
 $PCM SOLVNT=WATER $END
 $PCMCAV ALPHA=1 $END
 $DATA
Cl Anion MP2 6-311+G(d,p) VDV Calculation
C1
Cl 17 0.00000000 0.00000000 0.00000000
 $END
```

S12. Optimised Geometries (MP2/6-311+G(d,p))

Hydroxide Anion
O 8 0.00000000 0.00000000 0.00000000
H 1 0.96550676 0.00000000 0.00000000

Water
O 8 0.00000000 0.00000000 0.00000000
H 1 -0.75403990 -0.59420183 0.00000000
H 1 0.75250553 -0.59614379 0.00000000

Ethoxide Anion
C 6 0.00000000 0.00000000 0.00000000
C 6 -1.35865858 0.75622630 -0.00018254
O 8 -2.43068857 -0.04869850 -0.00023142
H 1 -1.29032566 1.45487795 -0.88985120
H 1 -1.29049648 1.45500148 0.88940194
H 1 0.86010729 0.69274213 0.00003458
H 1 0.05587483 -0.64302339 -0.88660062
H 1 0.05570424 -0.64290080 0.88670022

Ethanol
C 6 0.00000000 0.00000000 0.00000000
C 6 -1.27292962 0.82112560 -0.00056028
O 8 -2.37261449 -0.08970947 0.00016819
H 1 -3.17958646 0.43223511 -0.00019635
H 1 -1.30712120 1.46367895 -0.88993536
H 1 -1.30704029 1.46502964 0.88783847
H 1 0.87559674 0.65533417 -0.00052969
H 1 0.03817247 -0.63680001 -0.88665063
H 1 0.03824559 -0.63546203 0.88760749

Fluoride Anion
F 9 0.00000000 0.00000000 0.00000000

Hydrofluoric Acid
F 9 0.00000000 0.00000000 0.00000000
H 1 0.91704155 0.00000000 0.00000000

Methylacetamide Anion
C 6 0.00000000 0.00000000 0.00000000
N 7 -1.27193656 -0.69547953 -0.13070824
C 6 -2.29063875 0.08950319 0.19938860
O 8 -2.26168220 1.30062981 0.58957013
C 6 -3.66756326 -0.57406625 0.08692312
H 1 -3.58327967 -1.60910621 -0.25480816
H 1 -4.16529162 -0.54540374 1.06374933
H 1 -4.29010850 -0.00233714 -0.61186204
H 1 0.06115170 0.89600274 -0.64111896
H 1 0.18468080 0.35630226 1.02786468

H 1 0.81321050 -0.68211073 -0.28082216

Methylacetamide
C 6 0.00000000 0.00000000 0.00000000
N 7 1.33097259 -0.54060354 0.22591123
C 6 2.42561812 0.09296582 -0.29810167
O 8 2.34425250 1.18912138 -0.83903179
C 6 3.74330973 -0.64104436 -0.14330160
H 1 4.10805438 -0.91436452 -1.13645405
H 1 3.66598188 -1.53983091 0.47264273
H 1 4.46837686 0.04150451 0.30355290
H 1 1.42280027 -1.50953930 0.48870386
H 1 -0.02023221 1.04542479 0.30959446
H 1 -0.71486441 -0.56659222 0.59790784
H 1 -0.28335048 -0.04943759 -1.05596046

Methylmesylamide Anion
C 6 0.00000000 0.00000000 0.00000000
S 16 1.47442218 -0.94544896 -0.36265587
O 8 1.23768075 -2.29566290 0.23251598
O 8 1.55689919 -0.99738944 -1.85391442
N 7 2.55565253 -0.05689627 0.35570987
C 6 3.90453446 -0.59612111 0.22718679
H 1 4.25690198 -0.66496791 -0.81669436
H 1 4.02745398 -1.59551347 0.67961679
H 1 4.58377225 0.08367865 0.75409419
H 1 0.10210580 0.99534827 -0.43215321
H 1 -0.12966352 0.05362554 1.08084534
H 1 -0.83349779 -0.53445332 -0.46033688

Methylmesylamide
C 6 0.00000000 0.00000000 0.00000000
S 16 0.42342972 -1.71009705 -0.21701236
O 8 -0.57107131 -2.52224739 0.46727834
O 8 0.72877713 -1.90836149 -1.62734694
N 7 1.82207587 -1.83251391 0.69768081
C 6 3.09939791 -1.69566202 -0.01520064
H 1 3.89774383 -1.79916758 0.72129179
H 1 3.16439201 -0.69577388 -0.44789421
H 1 3.22780096 -2.43224373 -0.81281142
H 1 1.75514750 -2.68974091 1.24062891
H 1 0.81959982 0.61708763 -0.36972622
H 1 -0.18391841 0.17920165 1.05830606
H 1 -0.90059575 0.17893209 -0.58919959

Guaiacolate Anion
C 6 0.00000000 0.00000000 0.00000000
O 8 0.96750091 0.59166885 0.86033522
C 6 2.24995103 0.12992016 0.57623537
C 6 3.21787000 1.09513689 0.30210242

C 6 4.55033169 0.73759036 0.03615366
C 6 4.89238129 -0.62129878 0.10533809
C 6 3.92158078 -1.59159627 0.37117280
C 6 2.55709962 -1.28205956 0.71163042
O 8 1.69351863 -2.15545120 1.05967485
H 1 4.20432562 -2.64223882 0.44021497
H 1 5.91627864 -0.93404485 -0.10357579
H 1 5.30069466 1.49963010 -0.16181145
H 1 2.89342358 2.13484158 0.26336786
H 1 0.04797295 -1.09006643 0.06888842
H 1 0.16847089 0.32374000 -1.03810440
H 1 -0.97728961 0.36083407 0.33503899

Guaiacol
C 6 0.00000000 0.00000000 0.00000000
O 8 -0.96795125 1.03054221 0.15951194
C 6 -2.28446646 0.64422750 0.10946569
C 6 -2.75481266 -0.66970934 0.07764693
C 6 -4.13786300 -0.90659966 0.05151319
C 6 -5.03260393 0.16275037 -0.01218895
C 6 -4.55777461 1.48032914 0.01097561
C 6 -3.18730761 1.72322092 0.02647006
O 8 -2.72349757 3.00520966 0.03096396
H 1 -1.75834457 2.94570103 0.01576778
H 1 -5.23366426 2.32872013 -0.04001710
H 1 -6.10242920 -0.02122692 -0.03457816
H 1 -4.50161916 -1.92937616 0.03346657
H 1 -2.06571926 -1.50523811 0.13131957
H 1 -0.15768233 -0.53526712 -0.94208478
H 1 -0.03651711 -0.70438297 0.83721727
H 1 0.96761204 0.49974198 -0.01309796

Acetate Anion
C 6 0.00000000 0.00000000 0.00000000
C 6 1.55782939 0.04998555 -0.00510202
O 8 2.06325164 1.16527982 0.29229142
O 8 2.13137404 -1.02008271 -0.34240519
H 1 -0.35664801 0.27970055 -0.99885810
H 1 -0.41209808 0.71413629 0.71937226
H 1 -0.35845741 -1.01075513 0.21725842

Acetic Acid
C 6 0.00000000 0.00000000 0.00000000
C 6 1.48840236 0.19537874 0.08242245
O 8 2.06029670 1.20346901 0.42800300
O 8 2.14933009 -0.93349315 -0.28995800
H 1 3.09163478 -0.72459720 -0.20908721
H 1 -0.27779580 -0.26351614 -1.02280945
H 1 -0.50379413 0.91580295 0.30241378
H 1 -0.29654288 -0.82616517 0.64982362

Propionate Anion
C 6 0.00000000 0.00000000 0.00000000
C 6 1.30147574 0.86095815 0.03749125
O 8 1.19563064 2.02329166 -0.43882766
O 8 2.31625990 0.28276545 0.50985510
C 6 -1.28183694 0.82048715 0.12903214
H 1 -1.30879366 1.58771218 -0.64783156
H 1 -2.18142530 0.19417069 0.05180723
H 1 -1.30759411 1.33766723 1.09437301
H 1 0.00106999 -0.53263686 -0.96172392
H 1 0.06217611 -0.76121722 0.78566624

Propionic Acid
C 6 0.00000000 0.00000000 0.00000000
C 6 1.25366297 0.83854806 0.01089134
O 8 1.30248446 2.04734281 0.02978195
O 8 2.36670351 0.05693632 -0.00329045
H 1 3.11748165 0.66899969 0.00512964
C 6 -1.26715296 0.84554697 0.01406026
H 1 -1.30513800 1.50120460 -0.85811468
H 1 -2.15025241 0.20229091 0.00582625
H 1 -1.30276632 1.47541070 0.90513297
H 1 0.04522815 -0.64404237 -0.88466126
H 1 0.04737830 -0.66977786 0.86523977

Butyrate Anion
C 6 0.00000000 0.00000000 0.00000000
C 6 -1.42446384 0.63685745 0.00349771
O 8 -1.53372846 1.69702790 -0.67049414
O 8 -2.30162543 0.01350458 0.65795576
C 6 1.12183652 1.02705436 0.12353241
H 1 1.01057555 1.56011834 1.07711270
C 6 2.51861402 0.40594711 0.04530783
H 1 2.66015812 -0.33990581 0.83644596
H 1 3.31032576 1.15894244 0.14721929
H 1 2.65926040 -0.10280307 -0.91583930
H 1 0.98676166 1.77338353 -0.66479087
H 1 0.06628244 -0.74164560 0.80563458
H 1 0.11537651 -0.53740717 -0.95388786

Butyric Acid
C 6 0.00000000 0.00000000 0.00000000
C 6 -1.36910759 0.63165870 0.00375889
O 8 -1.60630216 1.81820367 0.01088752
O 8 -2.34638149 -0.31469656 -0.00192463
H 1 -3.18403642 0.17206135 0.00106634
C 6 1.12957928 1.02325512 0.00574619
H 1 1.02553394 1.66571404 0.88549744
C 6 2.50059881 0.34935865 0.00215083
H 1 2.62556891 -0.28752210 0.88366416

H 1 3.30356512 1.09133182 0.00619752
H 1 2.62564798 -0.27797507 -0.88616462
H 1 1.02572990 1.67537878 -0.86689260
H 1 0.06273993 -0.66206792 0.87197951
H 1 0.06257079 -0.65209581 -0.87947134

Formate Anion
C 6 0.00000000 0.00000000 0.00000000
O 8 -1.14190533 -0.52669260 -0.00185322
O 8 1.14204057 -0.52640100 -0.00199782
H 1 -0.00012535 1.13325613 0.00414326

Formic Acid
C 6 0.00000000 0.00000000 0.00000000
O 8 1.04005109 -0.60792235 0.00000000
O 8 -1.22771571 -0.55815495 0.00000000
H 1 -1.08804148 -1.51760480 0.00000000
H 1 -0.09468670 1.09205601 0.00000000

Nitrite Anion
N 7 0.00000000 0.00000000 0.00000000
O 8 -1.07473026 0.66794435 0.00000000
O 8 1.07458147 0.66818370 0.00000000

Nitrous Acid
N 7 0.00000000 0.00000000 0.00000000
O 8 -0.93757330 0.71658880 -0.01265396
O 8 1.20955107 0.74550597 -0.02105066
H 1 1.87635778 0.04290771 -0.00772865

Methylcarbonate Anion
C 6 0.00000000 0.00000000 0.00000000
O 8 1.20908791 -0.72350091 0.00008567
C 6 2.40783735 0.11634579 0.00115110
O 8 2.18878074 1.34406786 0.00199258
O 8 3.44247215 -0.56347872 0.00104539
H 1 -0.09914099 0.64234677 0.88364231
H 1 -0.80655306 -0.74328656 -0.00018352
H 1 -0.09901225 0.64251207 -0.88356029

Methylcarbonic Acid
C 6 0.00000000 0.00000000 0.00000000
O 8 1.25790719 -0.69611739 0.00079554
C 6 2.33451501 0.12497318 -0.00217026
O 8 2.30510916 1.32430180 -0.00526717
O 8 3.46507270 -0.60282996 -0.00114391
H 1 3.20917377 -1.53373580 0.00147438
H 1 -0.08494095 0.62501287 0.88943033
H 1 -0.75833938 -0.77974814 0.00256288
H 1 -0.08631416 0.62048741 -0.89245975

Chloride Anion
Cl 17 0.00000000 0.00000000 0.00000000

Hydrochloric Acid
Cl 17 0.00000000 0.00000000 0.00000000
H 1 1.27367038 0.00000000 0.00000000

Phosphinate Anion
P 15 0.00000000 0.00000000 0.00000000
H 1 0.00020235 0.92492951 1.09284823
H 1 -0.00037594 0.92529747 -1.09252706
O 8 1.33746454 -0.70997542 -0.00044670
O 8 -1.33733098 -0.71022722 0.00020857

Phosphinic Acid
P 15 0.00000000 0.00000000 0.00000000
H 1 -0.16503460 0.77993711 -1.15320035
H 1 -0.21211891 0.88793379 1.05669197
O 8 -1.40658690 -0.79746370 0.11390763
H 1 -1.42467977 -1.59563412 -0.42617097
O 8 1.25004784 -0.79675620 0.01355800

Dimethylphosphate Anion
P 15 0.00000000 0.00000000 0.00000000
O 8 -0.81788160 -1.36070375 -0.55671064
C 6 -2.05433082 -1.61975457 0.07671192
H 1 -1.92339028 -1.78515858 1.15246210
H 1 -2.47504368 -2.51856565 -0.38508170
H 1 -2.76015324 -0.79003657 -0.06437511
O 8 -0.46229474 1.21127764 -0.74397503
O 8 0.03522906 -0.09345791 1.50197244
O 8 1.47585210 -0.42451265 -0.61642401
C 6 2.12347850 -1.52423355 -0.00272511
H 1 3.08376247 -1.65539791 -0.51056169
H 1 1.53053332 -2.44051771 -0.11173700
H 1 2.29208904 -1.33989591 1.06367136

Dimethylphosphoric Acid
P 15 0.00000000 0.00000000 0.00000000
O 8 -0.83841648 -1.26055745 -0.51290322
C 6 -2.19215454 -1.41600184 -0.05128943
H 1 -2.22324211 -1.43153845 1.03992691
H 1 -2.53792333 -2.36602301 -0.45334695
H 1 -2.81530713 -0.60424289 -0.43446438
O 8 -0.52984702 1.19694182 -0.93203053
H 1 -0.47838140 2.03633370 -0.46091343
O 8 -0.05923119 0.27419926 1.45187663
O 8 1.42940397 -0.30215209 -0.63255988
C 6 2.20052735 -1.38491838 -0.07949257
H 1 3.17114935 -1.33975288 -0.56870099

H 1 1.71573510 -2.33866283 -0.29876192
H 1 2.31759197 -1.25758382 0.99896881

Methylhydrogenphosphonate Anion
P 15 0.00000000 0.00000000 0.00000000
O 8 -1.33590381 0.52333556 0.87856094
C 6 -2.10487365 1.54222089 0.27347754
H 1 -1.51730006 2.45322395 0.12026639
H 1 -2.95031965 1.75285420 0.93643450
H 1 -2.49993640 1.22802786 -0.70476369
O 8 0.58574508 1.20018653 -0.69843994
O 8 0.76594225 -0.92430957 0.89771508
H 1 -0.69623713 -0.76836879 -0.97360971

Monomethylphosphite
P 15 0.00000000 0.00000000 0.00000000
O 8 -1.22891644 0.61895655 0.82129387
C 6 -2.10571833 1.55576148 0.17566585
H 1 -1.58932593 2.50101921 0.00058369
H 1 -2.94361956 1.70259506 0.85376617
H 1 -2.47371207 1.15676734 -0.77540403
O 8 0.70910003 1.27558825 -0.70264816
H 1 1.54893825 1.48780098 -0.27799894
O 8 0.88086154 -0.86537647 0.80249907
H 1 -0.61220282 -0.56002369 -1.12191033

Nitrate Anion
N 7 0.00000000 0.00000000 0.00000000
O 8 0.15587816 -1.25269162 0.00000000
O 8 1.00692361 0.76134010 0.00000000
O 8 -1.16280184 0.49135116 0.00000000

Nitric Acid
N 7 0.00000000 0.00000000 0.00000000
O 8 -0.62211809 1.04329337 0.00000000
O 8 -0.77620296 -1.17810822 0.00000000
H 1 -1.68469441 -0.83419559 0.00000000
O 8 1.18609909 -0.20417239 0.00000000

Dimethylthiophosphate Anion
P 15 0.00000000 0.00000000 0.00000000
O 8 0.64501015 1.28038930 -0.85116333
C 6 1.36011240 2.24659604 -0.09964019
H 1 0.71919599 2.70742677 0.66287433
H 1 1.69158710 3.01668593 -0.80253537
H 1 2.22606162 1.80076680 0.39918091
O 8 -0.48596646 -0.96266894 -1.03461474
O 8 0.90723293 -0.31314539 1.15091585
S 16 -1.72386764 0.97271225 0.88331909
C 6 -2.61942203 1.32762880 -0.65604897

H 1 -2.78477306 0.40337828 -1.21232878
H 1 -2.05256787 2.02102724 -1.28167268
H 1 -3.58083028 1.77975411 -0.39506594

Dimethylthiophosphoric Acid
P 15 0.00000000 0.00000000 0.00000000
O 8 0.55670879 1.27921018 -0.81575012
C 6 1.15379367 2.33810290 -0.04320428
H 1 0.41809449 2.77001659 0.64117891
H 1 1.47552544 3.08920832 -0.76204523
H 1 2.00655946 1.96115016 0.52343820
O 8 -0.29552423 -0.98722188 -1.23617923
H 1 0.50261605 -1.19074030 -1.73943913
O 8 0.88176376 -0.46830906 1.08785729
S 16 -1.90482059 0.46543535 0.65827248
C 6 -2.63734919 1.02124680 -0.91355420
H 1 -2.70969486 0.19198316 -1.61615056
H 1 -2.05448549 1.83424476 -1.34651671
H 1 -3.63707237 1.38381317 -0.66909627

Trifluoroacetate Anion
C 6 0.00000000 0.00000000 0.00000000
C 6 1.57135744 -0.00541926 -0.00555257
O 8 2.07204654 1.08481885 0.33781328
O 8 2.06268784 -1.08247716 -0.40016483
F 9 -0.48379770 0.41830912 -1.20610383
F 9 -0.54922397 0.82546270 0.92390822
F 9 -0.55925371 -1.21456363 0.22033948

Trifluoroacetic Acid
C 6 0.00000000 0.00000000 0.00000000
C 6 1.53254159 0.09619672 0.14159698
O 8 2.09272409 0.94820949 0.77797861
O 8 2.10494717 -0.90142702 -0.54527019
H 1 3.06290080 -0.80542046 -0.43112300
F 9 -0.35387688 0.09092827 -1.28900965
F 9 -0.59226848 0.97940506 0.67312557
F 9 -0.43768684 -1.17318772 0.47654106

Thiocyanate Anion
C 6 0.00000000 0.00000000 0.00000000
S 16 1.66018648 -0.00021964 0.00000000
N 7 -1.19444143 0.00015784 0.00000000

Thiocyanic Acid (N-Protonated)
C 6 0.00000000 0.00000000 0.00000000
S 16 -1.56717742 0.07212851 0.00000000
N 7 1.19568180 -0.22103142 0.00000000
H 1 1.98999647 0.39916671 0.00000000

Methanesulphonate (Mesylate) Anion
C 6 0.00000000 0.00000000 0.00000000
S 16 1.80155279 -0.00049398 -0.00008663
O 8 2.16709097 1.43176243 -0.11114183
O 8 2.16640623 -0.81294003 -1.18504952
O 8 2.16654662 -0.62061873 1.29588327
H 1 -0.34912041 0.58474649 0.85279725
H 1 -0.34960674 -1.03075789 0.07991879
H 1 -0.34923114 0.44632652 -0.93269046

Methansulphonic Acid
C 6 0.00000000 0.00000000 0.00000000
S 16 1.73949525 -0.31342523 0.00692548
O 8 2.13387345 0.63287728 1.28494163
H 1 2.95948126 1.08523326 1.05733180
O 8 2.35832712 0.27112552 -1.16828805
O 8 1.96812513 -1.69434319 0.36168197
H 1 -0.40764468 -0.29098031 0.96743937
H 1 -0.42484681 -0.61679487 -0.79266733
H 1 -0.16726294 1.05691273 -0.20007553

***p*-Toluenesulphonate Anion**
S 16 0.00000000 0.00000000 0.00000000
O 8 0.37759601 1.11850946 0.89118930
C 6 -1.80628893 -0.00641604 0.05154664
C 6 -2.51060897 1.19081416 0.21925421
C 6 -3.90886340 1.19222079 0.19070050
C 6 -4.63126321 0.00837543 -0.02256665
C 6 -3.91130441 -1.18423350 -0.19042038
C 6 -2.51306032 -1.19463770 -0.16330832
H 1 -1.95534357 -2.11901242 -0.28527410
H 1 -4.45371343 -2.11531166 -0.35401861
C 6 -6.14099063 0.00683593 -0.00350359
H 1 -6.54093744 -0.78777904 -0.64180353
H 1 -6.53921714 0.96208349 -0.36090798
H 1 -6.52755676 -0.15548140 1.00997795
H 1 -4.44933886 2.12885912 0.32662351
H 1 -1.95100362 2.10585102 0.39228645
O 8 0.30663713 0.22892144 -1.42947744
O 8 0.37506642 -1.34183248 0.49667081

***p*-Toluenesulphonic Acid**
S 16 0.00000000 0.00000000 0.00000000
O 8 0.37767602 0.01148968 1.59420017
H 1 0.54920834 0.93010513 1.84999670
C 6 -1.76573156 0.02191231 0.04478024
C 6 -2.43645272 1.24760352 0.02169162
C 6 -3.83202720 1.25012375 0.08119129
C 6 -4.55952225 0.05388559 0.17387374
C 6 -3.85361179 -1.15915128 0.18894234

C 6 -2.45902591 -1.18845255 0.12530905
H 1 -1.91577335 -2.12826620 0.12157716
H 1 -4.40281314 -2.09630634 0.24346979
C 6 -6.06331654 0.07179363 0.27632891
H 1 -6.49753287 -0.82507345 -0.17324172
H 1 -6.48067163 0.94636380 -0.22958405
H 1 -6.37959322 0.10788283 1.32451680
H 1 -4.36404243 2.19819435 0.04920496
H 1 -1.87815114 2.17403198 -0.07310778
O 8 0.46724610 1.25401385 -0.56107616
O 8 0.43591646 -1.28467342 -0.48819184

Ethylsulphate Anion
C 6 0.00000000 0.00000000 0.00000000
C 6 1.34328973 0.70657441 0.03938227
O 8 2.34348318 -0.29797363 0.09585492
S 16 3.93022062 0.31084535 -0.00772869
O 8 4.01198701 1.26791061 1.10959794
O 8 4.70804196 -0.91837868 0.14858181
O 8 3.98609197 0.93536083 -1.34106098
H 1 1.41737035 1.35893746 0.91912519
H 1 1.48296741 1.32393992 -0.85769184
H 1 -0.06455835 -0.63826032 -0.88523490
H 1 -0.81632109 0.73110775 -0.03141805
H 1 -0.12331334 -0.62548774 0.88842221

Monoethylsulphuric Acid
C 6 0.00000000 0.00000000 0.00000000
C 6 -1.30386746 0.72192156 0.24787554
O 8 -2.34212142 -0.10116825 -0.35862566
S 16 -3.85807393 0.35753292 -0.10912857
O 8 -3.93964515 1.79044147 -0.12016879
O 8 -4.65962038 -0.50305085 -0.93288629
O 8 -4.07342264 -0.06508751 1.44445958
H 1 -4.26136926 -1.01522407 1.46942255
H 1 -1.32949648 1.70745336 -0.22121363
H 1 -1.51756919 0.82310341 1.31582233
H 1 -0.00668311 -0.98230282 0.47615580
H 1 0.82222530 0.58692413 0.41874809
H 1 0.16903973 -0.12497162 -1.07119248

Methylsulphate Anion
S 16 0.00000000 0.00000000 0.00000000
O 8 -1.43982081 -0.00150996 0.90145922
C 6 -2.60392410 -0.01877990 0.09484519
H 1 -2.63817837 -0.91853532 -0.53080266
H 1 -2.65142514 0.86679001 -0.54988398
H 1 -3.45544026 -0.01777330 0.78072340
O 8 -0.07258816 -1.24466902 -0.78533581
O 8 -0.09132361 1.22678900 -0.81108491

O 8 0.99699825 0.01871726 1.07034249

Monomethylsulphuric Acid
S 16 0.00000000 0.00000000 0.00000000
O 8 1.44151145 0.66710792 0.22568216
C 6 2.46124720 -0.18785296 0.79381256
H 1 2.67768079 -1.01362183 0.11606622
H 1 2.13777595 -0.56384468 1.76649790
H 1 3.32808914 0.45934927 0.90483616
O 8 -0.77138378 0.98911009 -0.69700424
O 8 0.15961418 -1.35766226 -0.43571293
O 8 -0.54644216 -0.10894910 1.52420273
H 1 -0.88637673 0.76101195 1.78181345

Dicyanamide Anion
N 7 0.00000000 0.00000000 0.00000000
C 6 -1.13337747 -0.68167043 -0.00493221
N 7 -2.21900206 -1.17068025 -0.00840610
C 6 1.13348488 -0.68148679 -0.00546882
N 7 2.21918925 -1.17031639 -0.00945367

Dicyanamidic Acid
N 7 0.00000000 0.00000000 0.00000000
C 6 1.17563702 -0.67797271 -0.03607594
N 7 2.20704202 -1.24090907 -0.02332909
C 6 -1.17564587 -0.67795899 -0.03605630
N 7 -2.20705815 -1.24088001 -0.02329476
H 1 0.00000174 0.94047944 -0.37642978

Tricyanomethanide Anion
C 6 0.00000000 0.00000000 0.00000000
C 6 -0.24000928 -1.39119507 0.00000000
N 7 -0.44131544 -2.55800243 0.00000000
C 6 -1.08480572 0.90345320 0.00000000
N 7 -1.99464847 1.66117991 0.00000000
C 6 1.32481263 0.48775033 0.00000000
N 7 2.43594440 0.89683518 0.00000000

Tricyanomethanidic Acid (Cyanoform)
C 6 0.00000000 0.00000000 0.00000000
C 6 -0.57452678 -1.28061055 0.45457743
N 7 -1.03485710 -2.30667690 0.79341918
C 6 -0.82176986 1.13780848 0.45472191
N 7 -1.48019993 2.04945772 0.79368220
C 6 1.39626322 0.14271751 0.45471326
N 7 2.51499699 0.25706794 0.79366745
H 1 0.00002836 0.00006516 -1.09905062

Triflate Anion
S 16 0.00000000 0.00000000 0.00000000

O 8 -0.30995562 -0.66363159 -1.27446167
C 6 1.85692238 -0.00000034 0.00000154
F 9 2.36018173 0.57753075 1.10911822
F 9 2.36018186 0.67175590 -1.05471411
F 9 2.36018105 -1.24928923 -0.05439909
O 8 -0.30995492 1.43553192 0.06251571
O 8 -0.30995645 -0.77190018 1.21195288

Triflic Acid
C 6 0.00000000 0.00000000 0.00000000
S 16 1.72400545 0.43531374 -0.51466034
O 8 1.63098594 1.21898320 -1.71153486
O 8 2.50956604 -0.76661336 -0.37956488
O 8 2.08527816 1.44985831 0.69001372
H 1 2.49503370 0.94780994 1.41217909
F 9 -0.77011078 1.07809477 0.00135968
F 9 -0.48671597 -0.89526188 -0.85005257
F 9 0.02749234 -0.52472094 1.22570943

Bistriflimide Anion
S 16 0.00000000 0.00000000 0.00000000
N 7 1.19919015 -0.75898583 0.74348751
S 16 2.39802215 -1.51762366 -0.00093317
C 6 3.69729694 -0.19340466 -0.05430300
F 9 4.02025029 0.22558859 1.17442389
F 9 3.28617881 0.86262372 -0.76226773
F 9 4.81319108 -0.67136588 -0.63173051
O 8 2.19174539 -1.87013847 -1.39879080
O 8 2.95731495 -2.50291931 0.91237864
C 6 -1.29930162 -1.32419237 -0.05336941
F 9 -2.41547214 -0.84595756 -0.63003579
F 9 -1.62166573 -1.74375831 1.17531690
F 9 -0.88852325 -2.37988806 -0.76202661
O 8 -0.55885355 0.98487278 0.91403676
O 8 0.20560602 0.35317476 -1.39778984

Bistriflimidic Acid
S 16 0.00000000 0.00000000 0.00000000
N 7 1.23779525 -0.89558931 0.70847780
H 1 1.24800057 -0.89125246 1.72692690
S 16 2.46119734 -1.79728380 -0.01702148
O 8 2.04767307 -2.17547798 -1.34002874
O 8 2.92066890 -2.70622554 1.00321111
C 6 3.77833256 -0.49790982 -0.19320357
F 9 4.04418304 0.01723480 1.00463851
F 9 3.36668554 0.46090188 -1.00685265
F 9 4.86912474 -1.07185138 -0.68428924
O 8 -0.43899689 0.91761621 1.02148203
O 8 0.38686367 0.36690127 -1.33420116
C 6 -1.32027490 -1.30072524 -0.13865868

F 9 -2.42075484 -0.73091328 -0.61264747
F 9 -1.56200686 -1.80559514 1.06862713
F 9 -0.92493601 -2.26647563 -0.95218167

Tetrafluoroborate Anion
B 5 0.00000000 0.00000000 0.00000000
F 9 -0.03113281 0.80803209 1.16085199
F 9 -1.14388751 -0.83204310 -0.02622996
F 9 1.16579864 -0.80135497 0.01435538
F 9 0.00922172 0.82536587 -1.14897711

Tetrafluoroboric Acid (Dissociated)
B 5 0.00000000 0.00000000 0.00000000
F 9 0.10878598 -0.10003346 -1.30870839
F 9 -0.19094719 1.18595299 0.55372865
F 9 0.17498527 -1.05764836 0.76505974
F 9 -2.53600430 -0.29935268 -0.05715290
H 1 -3.06167602 0.37890366 0.27327131

Hexafluorophosphate Anion
P 15 0.00000000 0.00000000 0.00000000
F 9 0.70543414 1.47380167 0.05186153
F 9 -0.42128361 0.25645567 -1.55857617
F 9 0.42121280 -0.25647897 1.55858723
F 9 -0.70540420 -1.47381470 -0.05186345
F 9 -1.41326241 0.65921693 0.49043739
F 9 1.41326376 -0.65917648 -0.49048197

Hexafluorophosphoric Acid (Dissociated)
P 15 0.00000000 0.00000000 0.00000000
F 9 -0.65433291 0.11767342 -1.44376557
F 9 -0.38954448 -1.53798601 -0.02237222
F 9 -0.11150630 1.57925436 0.10571470
F 9 -0.06748705 -0.05873936 1.57576146
F 9 1.51482038 -0.12237692 -0.30898876
F 9 -2.61814083 0.21404934 0.47452017
H 1 -3.16673953 0.29334340 -0.26081556

Tris(perfluoromethyl)trifluorophosphate Anion (FMP)
P 15 0.00000000 0.00000000 0.00000000
C 6 -1.92784497 -0.08038661 -0.11160293
F 9 -2.42407510 0.85872696 -0.95654032
F 9 -2.56416730 0.08726740 1.06794720
F 9 -2.35794153 -1.26274371 -0.60607449
F 9 -0.00004044 -0.17641287 -1.65343135
C 6 -0.00012699 1.94507244 -0.09405722
F 9 -0.00020407 2.46800352 -1.33673975
F 9 1.07476887 2.46893830 0.54661372
F 9 -1.07504425 2.46880151 0.54668957
C 6 1.92784872 -0.08014109 -0.11172337

F 9 2.42390543 0.85902928 -0.95669946
F 9 2.56422379 0.08760402 1.06778538
F 9 2.35806590 -1.26244701 -0.60621273
F 9 0.00003803 0.21547807 1.64054304
F 9 0.00011078 -1.63253335 0.24096980

Tris(perfluoromethyl)trifluorophosphoric Acid (Dissociated)
P 15 0.00000000 0.00000000 0.00000000
C 6 -1.72185655 -0.78849071 -0.15287766
F 9 -2.51982322 0.14275885 -0.70174373
F 9 -2.24646495 -1.16089465 1.00140658
F 9 -1.68311326 -1.84009166 -0.97664228
F 9 0.00005128 0.10177103 -1.64979073
C 6 -0.00261956 1.87946517 0.21000368
F 9 -0.00330071 2.54423404 -0.93574998
F 9 1.08320044 2.23110807 0.91068659
F 9 -1.08972441 2.22808021 0.91022407
C 6 1.72400142 -0.78388792 -0.15246117
F 9 2.51963388 0.14971084 -0.70077528
F 9 2.24917274 -1.15515592 1.00192408
F 9 1.68838936 -1.83532452 -0.97651560
F 9 -0.00000367 -0.15407032 1.62680024
F 9 0.00395454 -2.94506743 0.97317075
H 1 0.00276071 -3.72379535 0.48346795

Bis(oxalao)borate Anion
B 5 0.00000000 0.00000000 0.00000000
O 8 -0.88648123 0.17443668 1.16546234
C 6 -2.15491884 0.11457062 0.76597115
C 6 -2.15495272 -0.11474618 -0.76582864
O 8 -0.88653319 -0.17449950 -1.16540506
O 8 -3.13680694 -0.21910574 -1.46261579
O 8 -3.13673670 0.21884278 1.46282576
O 8 0.88645972 1.16546477 -0.17449823
C 6 2.15490509 0.76597123 -0.11476289
C 6 2.15496486 -0.76582826 0.11455188
O 8 0.88655341 -1.16540502 0.17443784
O 8 3.13683134 -1.46262020 0.21881659
O 8 3.13671111 1.46282582 -0.21913304

Bis(oxalato)boric Acid
B 5 0.00000000 0.00000000 0.00000000
O 8 0.95012379 1.03028074 0.89794965
C 6 2.11731487 0.71898082 0.62684099
C 6 2.24783425 -0.42745618 -0.37218462
O 8 1.03123606 -0.79232333 -0.69031791
O 8 3.32390545 -0.84102753 -0.73243065
O 8 3.16170248 1.29304345 1.12725173
H 1 3.93713864 0.84467654 0.73663811
O 8 -0.79610171 -0.72625547 0.92111823

C 6 -2.08658597 -0.31621466 0.75204464
C 6 -2.08642893 0.70201484 -0.41640726
O 8 -0.79586446 0.81325118 -0.84552092
O 8 -3.02911003 1.28259724 -0.86528259
O 8 -3.02941293 -0.68135233 1.38841186

Tetrachloroaluminate Anion
Al 13 0.00000000 0.00000000 0.00000000
Cl 17 2.14745910 0.07036388 -0.10894482
Cl 17 -0.71511466 -1.73356047 -1.05441025
Cl 17 -0.82205260 1.77444778 -0.89664000
Cl 17 -0.61025384 -0.11124892 2.06000602

Tetrachloroaluminic Acid (Dissociated)
Al 13 0.00000000 0.00000000 0.00000000
Cl 17 0.00919226 0.81524291 1.92533717
Cl 17 -0.31392701 1.33871772 -1.57118064
Cl 17 -0.53481863 -1.99769804 -0.25766530
Cl 17 2.49301136 -0.33085742 -0.23095915
H 1 2.86064093 0.83558716 0.15216572

Tetracyanoborate
B 5 0.00000000 0.00000000 0.00000000
C 6 -0.91970880 0.92023181 0.91985703
N 7 -1.59990838 1.60078581 1.60009980
C 6 0.92035826 0.91962648 -0.91981582
N 7 1.60100023 1.59974420 -1.60005467
C 6 -0.92014378 -0.91961271 -0.92004203
N 7 -1.60063929 -1.59972076 -1.60043785
C 6 0.91950771 -0.92026441 0.92002351
N 7 1.59950344 -1.60082787 1.60046232

Tetracyanoboric Acid
B 5 0.00000000 0.00000000 0.00000000
C 6 -0.42402374 0.68372646 1.35555351
N 7 -0.69966882 1.19786630 2.37861740
C 6 -0.36232302 0.85897574 -1.27109131
N 7 -0.59146324 1.50525191 -2.22858571
C 6 -0.46243666 -1.50285608 -0.11113761
N 7 -0.76702141 -2.63746486 -0.19398951
C 6 1.62644472 -0.05189061 0.03473391
N 7 2.78609700 -0.08889374 0.05948405
H 1 3.79194864 -0.12096844 0.08094225

[emim]-Carbene (Singlet)
C 6 0.00000000 0.00000000 0.00000000
N 7 1.32843053 -0.59225480 -0.04040798
C 6 1.60632381 -1.89081699 0.34070054
C 6 2.95088350 -2.06166088 0.13538825
N 7 3.41144658 -0.85987766 -0.36760902

C 6 2.43009681 0.09195672 -0.48901057
C 6 4.81294320 -0.58115547 -0.66031809
C 6 5.63176890 -0.42160017 0.61574158
H 1 5.21532626 0.38598780 1.22268605
H 1 6.67057854 -0.17975769 0.37194043
H 1 5.62230422 -1.34152468 1.20684574
H 1 4.81506975 0.33913951 -1.24632422
H 1 5.20584306 -1.39218375 -1.28284560
H 1 3.58451359 -2.92162215 0.29610357
H 1 0.85602286 -2.57584271 0.70755740
H 1 -0.67105921 -0.52144753 -0.68738750
H 1 0.10181210 1.04002979 -0.30611493
H 1 -0.40406005 -0.04905103 1.01426761

[emim]-Cation
C 6 0.00000000 0.00000000 0.00000000
N 7 1.34899418 -0.58547817 -0.00715411
C 6 1.67103401 -1.86428548 0.38070018
C 6 3.02489390 -2.01351544 0.18903546
N 7 3.49380862 -0.82404228 -0.31621904
C 6 2.46555816 0.03278762 -0.42803476
H 1 2.52571777 1.04623489 -0.79576844
C 6 4.90551393 -0.51410996 -0.63005735
C 6 5.75251176 -0.47975273 0.63371039
H 1 5.37207352 0.26701419 1.33441527
H 1 6.77899375 -0.21596289 0.36910952
H 1 5.76911236 -1.45374727 1.12748773
H 1 4.90156261 0.45108304 -1.14062971
H 1 5.24923899 -1.27272426 -1.33677770
H 1 3.67066193 -2.85996230 0.36606984
H 1 0.93051484 -2.55679036 0.75153740
H 1 -0.61240741 -0.49918594 -0.75091711
H 1 0.08278172 1.06090475 -0.23259212
H 1 -0.43149320 -0.12552475 0.99259438