Electronic Supplementary Material (ESI) for RSC Advances.

Structure of Amino Acid Ionic Liquids via Neutron Diffraction

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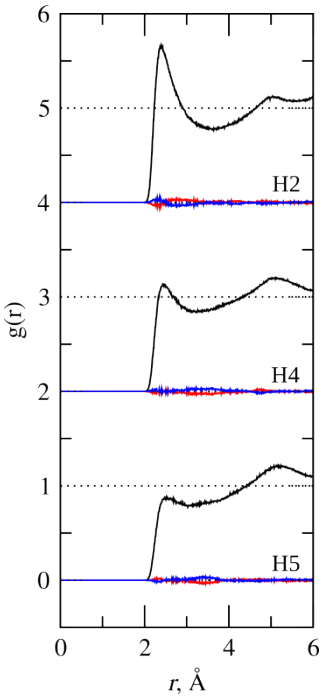
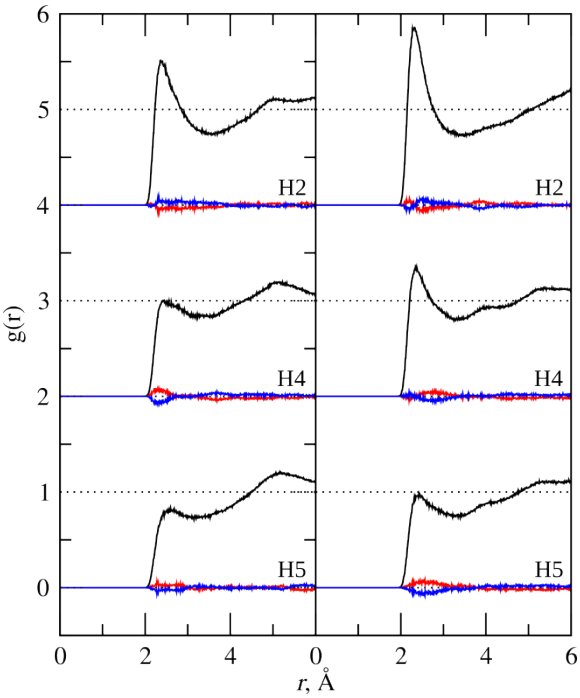
Supplementary Information

[C_2mim][Ala]

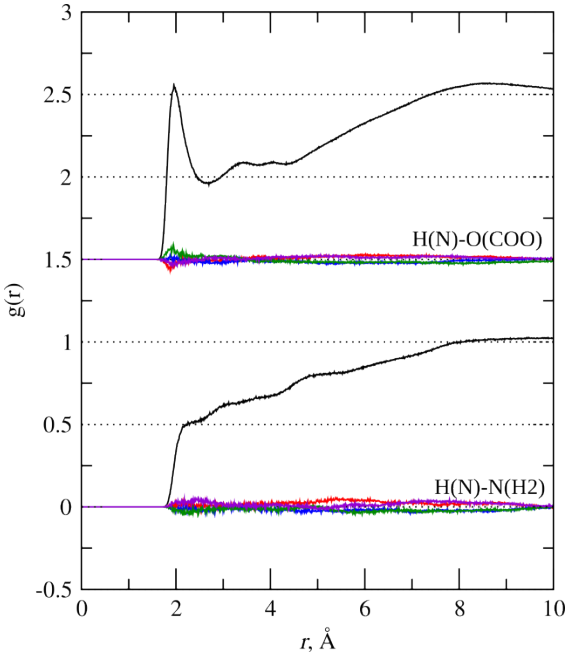


EMIM ring H to Ala N(H2) (black = original, red = R, blue = S)

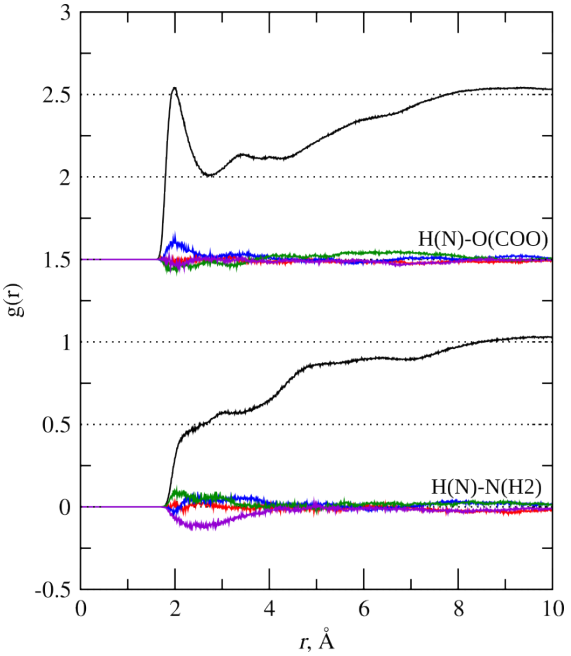
[C_2mim][Ser]



EMIM ring H to Ser N(H2) (left) and O(H) (right) (black = original, red = R, blue = S)



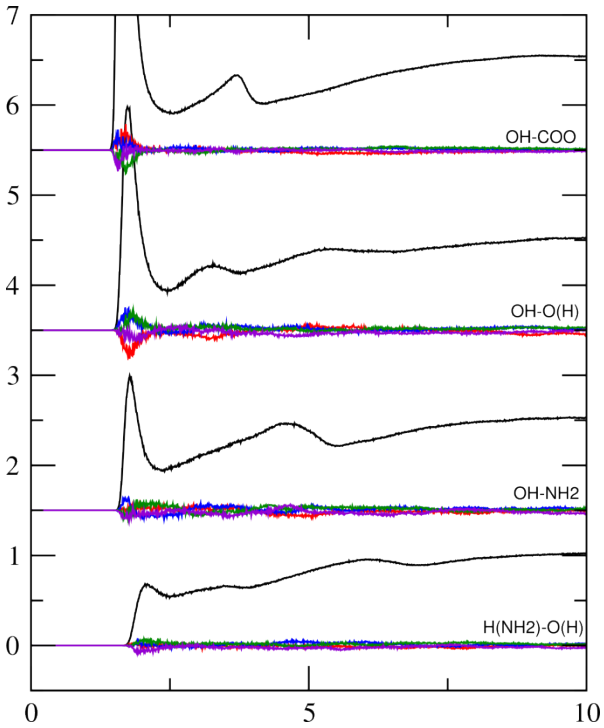
Differences in alaninate amine H to N(H_2) and O(COO) partials (black = original, red = RR (22), blue = RS (23), green = SR (32), and violet = SS



Differences in serinate amine H to N(H_2) and O(COO) partials (black = original, red = RR (22), blue = RS (23), green = SR (32), and violet = SS

(33))

(33))



Differences in serinate partials involving OH group (black = original, red = RR (22), blue = RS (23), green = SR (32), and violet = SS (33))

Molecular detail files for EPSR

1-ethyl-3-methylimidazolium cation

```
 .gmol           0
 atom            1  H1b  -0.305960000      0.449243009       2.35813594              1           2
 atom            2  C1    0.451999992     -9.32310000E-02    1.92300606              4           3           1          15          19
 atom            3  NA    0.123534001     -0.178635001      0.470872998             3           2           4           7
 atom            4  CR   -0.966162026      0.241712004      -9.68020037E-02         3           3           5          14
 atom            5  NA   -0.938925028     -1.55579997E-02  -1.42091703              3           4          10           6
 atom            6  CW    0.191183001     -0.724345982      -1.65256000             3           5           9           7
 atom            7  CW    0.867322981     -0.855059981     -0.489558011             3           3           6           8
 atom            8  HCW    1.78231502      -1.42358100     -0.285596997             1           7
 atom            9  HCW   0.414918989      -1.10908496      -2.61120892             1           6
 atom           10  C1    -1.89739096      0.304291010      -2.50104189             4           5          11          12          13
 atom           11  H1a   -1.49060202      0.863346994      -3.37342596             1          10
 atom           12  H1a   -2.23552990     -0.637015998      -2.93240094             1          10
 atom           13  H1a   -2.77735591      0.945151985      -2.17863202             1          10
 atom           14  HCR   -1.71167505      0.780197978      0.371327996             1           4
 atom           15  CE     1.82881105      0.515506029       2.39065289             4           2          16          17          18
 atom           16  HC     1.71436703       1.57997704       2.26757193             1          15
 atom           17  HC     2.70873690      0.137338996       1.93804801             1          15
 atom           18  HC     1.88502800      0.282270998       3.45725608             1          15
 atom           19  H1b   0.355385005      -1.06252301       2.36527205             1           2
bond HC  HC     1.83000
bond H1a H1a    1.83000
bond H1b H1b    1.83000
bond NA  C1     1.46600
bond NA  CR     1.31500
bond NA  CW     1.37800
bond CR  HCR    1.08000
bond CW  HCW    1.08000
bond CW  CW     1.34100
bond C1  H1     1.09000
bond C1  CE     1.52900
bond CE  HC     1.09000
bond HCR HCW    4.12000
bond HCW HCW    2.72000
bond C1  C1     5.02000
bond H1b C1     1.09000
bond C1  H1a    1.09000
angle NA  C1  H1   110.70000
angle NA  C1  CE   112.70000
angle H1  C1  CE   110.70000
angle H1  C1  H1   107.80000
angle C1  NA  CR   126.40000
angle C1  NA  CW   125.60000
angle CR  NA  CW   108.00000
angle NA  CR  NA   109.80000
angle NA  CR  HCR  125.10000
angle NA  CW  HCW  122.00000
angle NA  CW  CW   107.10000
angle HCW CW  CW   130.89999
angle C1  CE  HC   110.70000
angle HC  CE  HC   107.80000
angle NA  C1  H1b  110.70000
angle H1b C1  CE   110.70000
angle H1b C1  H1b  107.80000
angle NA  C1  H1a  110.70000
angle H1a C1  H1a  107.80000
rot   3   2
rot   5  10
rot   2  15
changelabel H1a H1
changelabel H1b H1
potential H1   0.12552E+00  0.25000E+01  0.10080E+01  0.13000E+00 H
potential C1   0.27614E+00  0.35000E+01  0.12011E+02 -0.17000E+00 C
potential NA   0.71128E+00  0.32500E+01  0.14007E+02  0.15000E+00 N
potential CR   0.29288E+00  0.35500E+01  0.12011E+02 -0.11000E+00 C
potential CW   0.29288E+00  0.35500E+01  0.12011E+02 -0.13000E+00 C
potential HCW  0.12552E+00  0.24200E+01  0.10080E+01  0.21000E+00 H
potential HCR  0.12552E+00  0.24200E+01  0.10080E+01  0.21000E+00 H
potential CE   0.27614E+00  0.35000E+01  0.12011E+02 -0.50000E-01 C
potential HC   0.12552E+00  0.25000E+01  0.10080E+01  0.60000E-01 H
temperature  0.300000E+03
vibtemp  0.650000E+02
angtemp  0.200000E+01
dihtemp  0.000000E+00
ecoredcore    1.00000    1.00000
density  0.100000E+00
```

Glycinate anion

```
.gmol           0
 atom            1  C1A  -0.283919990     -0.482041001      -5.67639992E-02          4           2           3           4           9
 atom            2  NH2  -0.674108028     -0.989943981      -1.36861205              3           1           7           8
 atom            3  COA    1.01859999      -1.06746697      0.544483006              3           1           5           6
 atom            4  H1A   -1.08283305     -0.691254973      0.651966989              1           1
 atom            5  OA     1.47298503      -2.07615805      -1.19519997E-02          1           3
 atom            6  OA     1.44237900     -0.468358010       1.53997505              1           3
 atom            7  HN    -3.37460004E-02 -0.628225982      -2.04932499              1           2
 atom            8  HN   -0.486234993      -1.97507000      -1.36065698              1           2
 atom            9  H1A  -0.193293005      0.598730028      -9.99090001E-02          1           1
bond C1A NH2    1.45985
bond C1A COA    1.54945
bond C1A H1A    1.08827
bond NH2 HN     1.00213
bond COA OA     1.23836
angle NH2 C1A COA  116.22729
angle NH2 C1A H1A  108.79141
angle COA C1A H1A  106.96436
angle H1A C1A H1A  106.17678
angle C1A NH2 HN   108.30218
angle HN  NH2 HN   103.90028
angle C1A COA OA   116.22171
angle OA  COA OA   129.08961
rot   1   2
rot   1   3
potential C1A  0.66000E-01  0.35000E+01  0.12011E+02  0.33800E+00 C
potential NH2  0.17000E+00  0.33000E+01  0.14007E+02 -0.11190E+01 N
potential COA  0.10500E+00  0.37500E+01  0.12011E+02  0.95300E+00 C
potential H1A  0.30000E-01  0.25000E+01  0.10080E+01 -0.39500E-01 H
potential OA   0.21000E+00  0.29600E+01  0.15999E+02 -0.92150E+00 O
potential HN   0.15000E-01  0.20000E+01  0.10080E+01  0.37500E+00 H
temperature  0.300000E+03
vibtemp  0.650000E+02
angtemp  0.200000E+01
dihtemp  0.000000E+00
ecoredcore    1.00000    1.00000
density  0.100000E+00
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Alaninate anion (R)

```
.gmol           0
 atom            1  C1A  -0.339547008     -0.488074005      -8.59439969E-02          4           2           3           4           5
 atom            2  C2A  -0.336870015      1.03524196      -0.177248001              4           1           6           7          12
 atom            3  NH2  -0.664905012     -1.06275904      -1.39094806              3           1          10          11
 atom            4  COA   0.974878013      -1.03341305      0.550190985              3           1           8           9
 atom            5  H1A   -1.13522995     -0.776373029      0.600166023              1           1
 atom            6  H2A   0.445879012      1.37729394      -0.854586005              1           2
 atom            7  H2A   -1.29024899      1.39827204      -0.556630015              1           2
 atom            8  OA     1.52009702      -1.97398806      -4.19650003E-02          1           4
 atom            9  OA     1.31215501     -0.483065009       1.60529602              1           4
 atom           10  HN    -3.42019983E-02 -0.676191986      -2.06878304              1           3
 atom           11  HN   -0.406165987      -2.03033495      -1.35106599              1           3
 atom           12  H2A  -0.142542005       1.46719205      0.795212984              1           2
bond C1A C2A    1.52605
bond C1A NH2    1.46259
bond C1A COA    1.55877
bond C1A H1A    1.08948
bond C2A H2A    1.09018
bond NH2 HN     1.00333
bond COA OA     1.23798
bond OA  OA     2.23100
angle C2A C1A NH2  109.82971
angle C2A C1A COA  111.84901
angle C2A C1A H1A  107.64417
angle NH2 C1A COA  114.47198
angle NH2 C1A H1A  107.18539
angle COA C1A H1A  105.44217
angle C1A C2A H2A  110.58695
angle H2A C2A H2A  107.92091
angle C1A NH2 HN   108.15392
angle HN  NH2 HN   103.68172
angle C1A COA OA   115.62500
angle OA  COA OA   128.75000
rot   1   2
rot   1   3
rot   1   4
potential C1A  0.66000E-01  0.35000E+01  0.12011E+02  0.63600E+00 C
potential C2A  0.66000E-01  0.35000E+01  0.12011E+02 -0.42400E+00 C
potential NH2  0.17000E+00  0.33000E+01  0.14007E+02 -0.11930E+01 N
potential COA  0.10500E+00  0.37500E+01  0.12011E+02  0.80900E+00 C
potential H1A  0.30000E-01  0.25000E+01  0.10080E+01 -0.70000E-01 H
potential H2A  0.30000E-01  0.25000E+01  0.10080E+01  0.77000E-01 H
potential OA   0.21000E+00  0.29600E+01  0.15999E+02 -0.87650E+00 O
potential HN   0.15000E-01  0.20000E+01  0.10080E+01  0.38200E+00 H
temperature  0.300000E+03
vibtemp  0.650000E+02
angtemp  0.200000E+01
dihtemp  0.000000E+00
ecoredcore    1.00000    1.00000
density  0.100000E+00
```

Alaninate anion (S)

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.gmol           0
 atom            1  C1A   -6.66190013E-02 -0.387836993     -0.655815005             4           2           3           4           5
 atom            2  C2A  -0.394439995       1.01846397     -0.162169993             4           1           6           7          12
 atom            3  NH2   -1.14435005      -1.30613804     -0.289238006             3           1          10          11
 atom            4  COA    1.35323203     -0.845167994     -0.203437001             3           1           8           9
 atom            5  H1A   -2.78140008E-02 -0.355120003      -1.74411595             1           1
 atom            6  H2A  -0.444429994       1.04059398      0.926634014             1           2
 atom            7  H2A   -1.35805798       1.34546196     -0.548390985             1           2
 atom            8  OA     1.43223202      -1.97864103      0.288080990             1           4
 atom            9  OA     2.25816107      -3.01089995E-02 -0.419467002             1           4
 atom           10  HN    -1.30135298      -1.22549796      0.698450029             1           3
 atom           11  HN   -0.779958010      -2.23375297     -0.396423012             1           3
 atom           12  H2A   0.376693010       1.71154702     -0.470411986             1           2
bond C1A C2A    1.52605
bond C1A NH2    1.46259
bond C1A COA    1.55877
bond C1A H1A    1.08948
bond C2A H2A    1.09018
bond NH2 HN     1.00333
bond COA OA     1.23798
bond OA  OA     2.23100
angle C2A C1A NH2  109.82971
angle C2A C1A COA  111.84901
angle C2A C1A H1A  107.64417
angle NH2 C1A COA  114.47198
angle NH2 C1A H1A  107.18539
angle COA C1A H1A  105.44217
angle C1A C2A H2A  110.58695
angle H2A C2A H2A  107.92091
angle C1A NH2 HN   108.15392
angle HN  NH2 HN   103.68172
angle C1A COA OA   115.62500
angle OA  COA OA   128.75000
rot   1   2
rot   1   3
rot   1   4
potential C1A  0.66000E-01  0.35000E+01  0.12011E+02  0.63600E+00 C
potential C2A  0.66000E-01  0.35000E+01  0.12011E+02 -0.42400E+00 C
potential NH2  0.17000E+00  0.33000E+01  0.14007E+02 -0.11930E+01 N
potential COA  0.10500E+00  0.37500E+01  0.12011E+02  0.80900E+00 C
potential H1A  0.30000E-01  0.25000E+01  0.10080E+01 -0.70000E-01 H
potential H2A  0.30000E-01  0.25000E+01  0.10080E+01  0.77000E-01 H
potential OA   0.21000E+00  0.29600E+01  0.15999E+02 -0.87650E+00 O
potential HN   0.15000E-01  0.20000E+01  0.10080E+01  0.38200E+00 H
temperature  0.300000E+03
vibtemp  0.650000E+02
angtemp  0.200000E+01
dihtemp  0.000000E+00
ecoredcore    1.00000    1.00000
density  0.100000E+00
```

Serinate anion (R)

```
.gmol           0
 atom            1  C1A  -0.382730991     -0.552901030     -0.141111001             4           2           3           4           5
 atom            2  C2A  -0.454566985      0.974842012     -0.161896005             4           1           6           7           8
 atom            3  NH2  -0.579509020      -1.05763495      -1.49681902             3           1          11          12
 atom            4  COA   0.904227018      -1.08857095      0.550917983             3           1           9          10
 atom            5  H1A   -1.21638501     -0.903473973      0.466179013             1           1
 atom            6  OH   -0.456671000       1.54265404       1.11350703             2           2          13
 atom            7  H2A   0.383946002       1.36299503     -0.748341978             1           2
 atom            8  H2A   -1.36864698       1.27851903     -0.662526011             1           2
 atom            9  OA     1.39062202      -2.11846495       8.34690034E-02         1           4
 atom           10  OA     1.29195094     -0.432900995       1.53711700             1           4
 atom           11  HN    0.107897997     -0.639487028      -2.09681892             1           3
 atom           12  HN   -0.331212997      -2.02839708      -1.48083305             1           3
 atom           13  HO    0.215193003       1.06305301       1.59899902             1           6
bond C1A C2A    1.52957
bond C1A NH2    1.45994
bond C1A COA    1.55631
bond C1A H1A    1.08935
bond C2A OH     1.39609
bond C2A H2A    1.09439
bond NH2 HN     1.00368
bond COA OA     1.23117
bond OH  HO     0.95766
angle C2A C1A NH2  109.04798
angle C2A C1A COA  112.87109
angle C2A C1A H1A  107.04173
angle NH2 C1A COA  113.91470
angle NH2 C1A H1A  107.65420
angle COA C1A H1A  105.91276
angle C1A C2A OH   113.19651
angle C1A C2A H2A  108.99889
angle OH  C2A H2A  110.27004
angle H2A C2A H2A  107.38698
angle C1A NH2 HN   108.58881
angle HN  NH2 HN   104.08822
angle C1A COA OA   116.47375
angle OA  COA OA   128.14915
angle C2A OH  HO   104.97440
rot   1   2
rot   1   3
rot   1   4
```

```
rot   2   6
potential C1A  0.66000E-01  0.35000E+01  0.12011E+02  0.31100E+00 C
potential C2A  0.66000E-01  0.35000E+01  0.12011E+02  0.30700E+00 C
potential NH2  0.17000E+00  0.33000E+01  0.14007E+02 -0.12080E+01 N
potential COA  0.10500E+00  0.37500E+01  0.12011E+02  0.83400E+00 C
potential H1A  0.30000E-01  0.25000E+01  0.10080E+01  0.11000E-01 H
potential OH   0.17000E+00  0.31200E+01  0.15999E+02 -0.83800E+00 O
potential H2A  0.30000E-01  0.25000E+01  0.10080E+01  0.25000E-02 H
potential OA   0.21000E+00  0.29600E+01  0.15999E+02 -0.85400E+00 O
potential HN   0.15000E-01  0.20000E+01  0.10080E+01  0.40600E+00 H
potential HO   0.15000E-01  0.15000E+01  0.10080E+01  0.47400E+00 H
temperature  0.300000E+03
vibtemp  0.650000E+02
angtemp  0.200000E+01
dihtemp  0.000000E+00
ecoredcore    1.00000    1.00000
density  0.100000E+00
```

Serinate anion (L)

```
.gmol           0
 atom            1  C1A  -0.181435004     -0.480704993     -0.491263002             4           2           3           4           5
 atom            2  C2A  -0.597853005      0.910414994      -1.06680002E-02         4           1           6           7           8
 atom            3  NH2   -1.22885501      -1.43736696     -0.146107003             3           1          11          12
 atom            4  COA    1.23613095     -0.891927004       2.20600003E-03         3           1           9          10
 atom            5  H1A  -0.118519001     -0.437483013      -1.57793403             1           1
 atom            6  OH    0.255755007       1.92308795     -0.452163011            2           2          13
 atom            7  H2A  -0.650578022      0.908726990       1.08244801            1           2
 atom            8  H2A   -1.59375203       1.12916195     -0.383127987            1           2
 atom            9  OA     1.40116000      -2.08300900      0.266510010            1           4
 atom           10  OA     2.07410097       2.93649994E-02   4.51989993E-02        1           4
 atom           11  HN    -1.38786697      -1.39432597      0.843962014            1           3
 atom           12  HN    -0.843066990     -2.35073900     -0.291729987            1           3
 atom           13  HO     1.13889205       1.57503295     -0.325489014            1           6
bond C1A C2A    1.52957
bond C1A NH2    1.45994
bond C1A COA    1.55631
bond C1A H1A    1.08935
bond C2A OH     1.39609
bond C2A H2A    1.09439
bond NH2 HN     1.00368
bond COA OA     1.23117
bond OH  HO     0.95766
angle C2A C1A NH2  109.04798
angle C2A C1A COA  112.87109
angle C2A C1A H1A  107.04173
angle NH2 C1A COA  113.91470
angle NH2 C1A H1A  107.65420
angle COA C1A H1A  105.91276
angle C1A C2A OH   113.19651
angle C1A C2A H2A  108.99889
angle OH  C2A H2A  110.27004
angle H2A C2A H2A  107.38698
angle C1A NH2 HN   108.58881
angle HN  NH2 HN   104.08822
angle C1A COA OA   116.47375
angle OA  COA OA   128.14915
angle C2A OH  HO   104.97440
rot   1   2
rot   1   3
rot   1   4
rot   2   6
potential C1A  0.66000E-01  0.35000E+01  0.12011E+02  0.31100E+00 C
potential C2A  0.66000E-01  0.35000E+01  0.12011E+02  0.30700E+00 C
potential NH2  0.17000E+00  0.33000E+01  0.14007E+02 -0.12080E+01 N
potential COA  0.10500E+00  0.37500E+01  0.12011E+02  0.83400E+00 C
potential H1A  0.30000E-01  0.25000E+01  0.10080E+01  0.11000E-01 H
potential OH   0.17000E+00  0.31200E+01  0.15999E+02 -0.83800E+00 O
potential H2A  0.30000E-01  0.25000E+01  0.10080E+01  0.25000E-02 H
potential OA   0.21000E+00  0.29600E+01  0.15999E+02 -0.85400E+00 O
potential HN   0.15000E-01  0.20000E+01  0.10080E+01  0.40600E+00 H
potential HO   0.15000E-01  0.15000E+01  0.10080E+01  0.47400E+00 H
temperature  0.300000E+03
vibtemp  0.650000E+02
angtemp  0.200000E+01
dihtemp  0.000000E+00
ecoredcore    1.00000    1.00000
density  0.100000E+00
```