Electronic Supplementary Material (ESI) for RSC Advances.

Computational analysis of the solvation of coffee ingredients in aqueous ionic liquid mixtures

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Abstract

CONTENTS

Force field of the coffee ingredients 2

Force field of the solvents 16

Hydrogen bonds and extraction yields 22

FORCE FIELD OF THE COFFEE INGREDIENTS

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*============================================================
*. Force field of the solute species
*============================================================
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READ RTF CARD
*.............................................................
*. Topology of the solutes
*.............................................................
*
   99     1

MASS  101 C5A        12.011
MASS  102 C5B        12.011
MASS  103 C=C        12.011
MASS  104 C=O        12.011
MASS  105 CB         12.011
MASS  106 CR         12.011
MASS  107 HCMM        1.008
MASS  108 HOCC        1.008
MASS  109 HOCO        1.008
MASS  110 N5B        14.007
MASS  111 NC=O       14.007
MASS  112 NPYL       14.007
MASS  113 O=C        15.999
MASS  114 OR         15.999

!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
! caffeine
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
RESIDUE CAFF  0.00000
GROUP
ATOM     N1   NPYL    0.16234
ATOM     C1     CR   -0.27493
ATOM    H11   HCMM    0.13334
ATOM    H12   HCMM     0.1324
ATOM    H13   HCMM    0.10401
ATOM     C2    C5A    0.07055
ATOM     H2   HCMM    0.12982
ATOM     N3    N5B   -0.47609
ATOM     C4    C5B    0.46692
ATOM     N5   NC=O   -0.35029
ATOM     C5     CR    0.15421
ATOM    H51   HCMM    0.02559
ATOM    H52   HCMM    0.02849
ATOM    H53   HCMM    0.00615
ATOM     C6    C=O    0.65534
ATOM     O6    O=C   -0.51422
ATOM     N7   NC=O   -0.38795
ATOM     C7     CR    0.02136
ATOM    H71   HCMM    0.05432
ATOM    H72   HCMM    0.05368
ATOM    H73   HCMM    0.05659
ATOM     C8    C=O    0.62056
```

```
ATOM      O8     O=C     -0.4932
ATOM      C9     C5A    -0.37899
BOND      C1      N1
BOND      C1     H11
BOND      C1     H12
BOND      C1     H13
BOND      N1      C9
BOND      N1      C2
BOND      C2      N3
BOND      C2      H2
BOND      N3      C4
BOND      C4      N5
BOND      C4      C9
BOND      N5      C5
BOND      C5     H51
BOND      C5     H52
BOND      C5     H53
BOND      C6      N5
BOND      C6      O6
BOND      N7      C6
BOND      N7      C7
BOND      C7     H71
BOND      C7     H72
BOND      C7     H73
BOND      C8      N7
BOND      C8      O8
BOND      C9      C8
ANGL      C1      N1      C2
ANGL      C1      N1      C9
ANGL      C2      N1      C9
ANGL      C2      N3      C4
ANGL      C4      C9      C8
ANGL      C4      C9      N1
ANGL      C4      N5      C5
ANGL      C4      N5      C6
ANGL      C5      N5      C6
ANGL      C6      N7      C7
ANGL      C6      N7      C8
ANGL      C7      N7      C8
ANGL      C8      C9      N1
ANGL      C9      C4      N3
ANGL      C9      C4      N5
ANGL      C9      C8      N7
ANGL      C9      C8      O8
ANGL     H11      C1     H12
ANGL     H11      C1     H13
ANGL     H11      C1      N1
ANGL     H12      C1     H13
ANGL     H12      C1      N1
ANGL     H13      C1      N1
ANGL      H2      C2      N1
ANGL      H2      C2      N3
ANGL     H51      C5     H52
ANGL     H51      C5     H53
ANGL     H51      C5      N5
ANGL     H52      C5     H53
ANGL     H52      C5      N5
```

```
ANGL    H53     C5      N5
ANGL    H71     C7     H72
ANGL    H71     C7     H73
ANGL    H71     C7      N7
ANGL    H72     C7     H73
ANGL    H72     C7      N7
ANGL    H73     C7      N7
ANGL     N1     C2      N3
ANGL     N3     C4      N5
ANGL     N5     C6      N7
ANGL     N5     C6      O6
ANGL     N7     C6      O6
ANGL     N7     C8      O8
DIHE     C1     N1      C2      H2
DIHE     C1     N1      C2      N3
DIHE     C1     N1      C9      C4
DIHE     C1     N1      C9      C8
DIHE     C2     N1      C1     H11
DIHE     C2     N1      C1     H12
DIHE     C2     N1      C1     H13
DIHE     C2     N1      C9      C4
DIHE     C2     N1      C9      C8
DIHE     C2     N3      C4      C9
DIHE     C2     N3      C4      N5
DIHE     C4     C9      C8      N7
DIHE     C4     C9      C8      O8
DIHE     C4     N3      C2      H2
DIHE     C4     N3      C2      N1
DIHE     C4     N5      C5     H51
DIHE     C4     N5      C5     H52
DIHE     C4     N5      C5     H53
DIHE     C4     N5      C6      N7
DIHE     C4     N5      C6      O6
DIHE     C5     N5      C4      C9
DIHE     C5     N5      C4      N3
DIHE     C5     N5      C6      N7
DIHE     C5     N5      C6      O6
DIHE     C6     N5      C4      C9
DIHE     C6     N5      C4      N3
DIHE     C6     N5      C5     H51
DIHE     C6     N5      C5     H52
DIHE     C6     N5      C5     H53
DIHE     C6     N7      C7     H71
DIHE     C6     N7      C7     H72
DIHE     C6     N7      C7     H73
DIHE     C6     N7      C8      C9
DIHE     C6     N7      C8      O8
DIHE     C7     N7      C6      N5
DIHE     C7     N7      C6      O6
DIHE     C7     N7      C8      C9
DIHE     C7     N7      C8      O8
DIHE     C8     C9      C4      N3
DIHE     C8     C9      C4      N5
DIHE     C8     N7      C6      N5
DIHE     C8     N7      C6      O6
DIHE     C8     N7      C7     H71
DIHE     C8     N7      C7     H72
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DIHE     C8     N7     C7    H73
DIHE     C9     N1     C1    H11
DIHE     C9     N1     C1    H12
DIHE     C9     N1     C1    H13
DIHE     C9     N1     C2     H2
DIHE     C9     N1     C2     N3
DIHE     N1     C9     C4     N3
DIHE     N1     C9     C4     N5
DIHE     N1     C9     C8     N7
DIHE     N1     C9     C8     O8
IMPR     N1     C2     C9     C1
IMPR     C2     N3     N1     H2
IMPR     C9     C4     N1     C8
IMPR     C8     N7     C9     O8
IMPR     N7     C6     C8     C7
IMPR     C4     C9     N3     N5
IMPR     C6     N5     N7     O6
IMPR     N5     C6     C4     C5
IMPR     C1    H11     N1    H12
IMPR     C1    H11     N1    H13
IMPR     C5    H51     N5    H52
IMPR     C5    H51     N5    H53
IMPR     C7    H71     N7    H72
IMPR     C7    H71     N7    H73
PATCHING FIRST NONE LAST NONE

!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
! gallic acid
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
RESIDUE  GAL  0.00000
GROUP
ATOM     O3     OR      -0.65
ATOM     H5   HOCO        0.5
ATOM     C6    C=O     0.6338
ATOM     O4    O=C      -0.57
ATOM      C     CB     0.0862
ATOM     C1     CB      -0.15
ATOM      H   HCMM       0.15
ATOM     C2     CB     0.0825
ATOM     O2     OR    -0.5325
ATOM     H4   HOCC       0.45
ATOM     C3     CB     0.0825
ATOM     O1     OR    -0.5325
ATOM     H3   HOCC       0.45
ATOM     C4     CB     0.0825
ATOM      O     OR    -0.5325
ATOM     H2   HOCC       0.45
ATOM     C5     CB      -0.15
ATOM     H1   HCMM       0.15
BOND      C     C1
BOND      C     C5
BOND      C     C6
BOND     C1     C2
BOND     C1      H
BOND     C2     C3
BOND     C2     O2
BOND     C3     C4
```

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BOND     C3     O1
BOND     C4     C5
BOND     C4      O
BOND     C5     H1
BOND      O     H2
BOND     O1     H3
BOND     O2     H4
BOND     C6     O3
BOND     C6     O4
BOND     O3     H5
ANGL      C     C1     C2
ANGL      C     C1      H
ANGL      C     C5     C4
ANGL      C     C5     H1
ANGL      C     C6     O3
ANGL      C     C6     O4
ANGL     C1      C     C5
ANGL     C1      C     C6
ANGL     C1     C2     C3
ANGL     C1     C2     O2
ANGL     C2     C1      H
ANGL     C2     C3     C4
ANGL     C2     C3     O1
ANGL     C2     O2     H4
ANGL     C3     C2     O2
ANGL     C3     C4     C5
ANGL     C3     C4      O
ANGL     C3     O1     H3
ANGL     C4     C3     O1
ANGL     C4     C5     H1
ANGL     C4      O     H2
ANGL     C5      C     C6
ANGL     C5     C4      O
ANGL     C6     O3     H5
ANGL     O3     C6     O4
DIHE      C     C1     C2     C3
DIHE      C     C1     C2     O2
DIHE      C     C5     C4     C3
DIHE      C     C5     C4      O
DIHE      C     C6     O3     H5
DIHE     C1      C     C5     C4
DIHE     C1      C     C5     H1
DIHE     C1      C     C6     O3
DIHE     C1      C     C6     O4
DIHE     C1     C2     C3     C4
DIHE     C1     C2     C3     O1
DIHE     C1     C2     O2     H4
DIHE     C2     C1      C     C5
DIHE     C2     C1      C     C6
DIHE     C2     C3     C4     C5
DIHE     C2     C3     C4      O
DIHE     C2     C3     O1     H3
DIHE     C3     C2     C1      H
DIHE     C3     C2     O2     H4
DIHE     C3     C4     C5     H1
DIHE     C3     C4      O     H2
DIHE     C4     C3     C2     O2
```

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DIHE     C4     C3     O1     H3
DIHE     C4     C5      C     C6
DIHE     C5      C     C1      H
DIHE     C5      C     C6     O3
DIHE     C5      C     C6     O4
DIHE     C5     C4     C3     O1
DIHE     C5     C4      O     H2
DIHE     C6      C     C1      H
DIHE     C6      C     C5     H1
DIHE      H     C1     C2     O2
DIHE     H1     C5     C4      O
DIHE     H5     O3     C6     O4
DIHE      O     C4     C3     O1
DIHE     O1     C3     C2     O2
IMPR      C     C1     C5     C6
IMPR     C1     C2      C      H
IMPR     C2     C3     C1     O2
IMPR     C3     C4     C2     O1
IMPR     C4     C5     C3      O
IMPR     C6     O3      C     O4
IMPR     C5     C4      C     H1
PATCHING FIRST NONE LAST NONE

!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
! quercetin
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
RESIDUE  QUE 0.0000
GROUP
ATOM     C5     CB      -0.15
ATOM     H1   HCMM       0.15
ATOM      C     CB      0.082
ATOM      O     OR     -0.532
ATOM     H2   HOCC       0.45
ATOM     C1     CB      -0.15
ATOM      H   HCMM       0.15
ATOM     C2     CB      0.082
ATOM     O1     OR     -0.532
ATOM     H3   HOCC       0.45
ATOM     C3     CB      0.086
ATOM     C4     CB      0.082
ATOM     O2     OR     -0.159
ATOM     C6    C=O      0.469
ATOM     O3    O=C     -0.569
ATOM     C7    C=C      0.091
ATOM     O4     OR     -0.526
ATOM     H4   HOCC       0.45
ATOM     C8    C=C      0.048
ATOM     C9     CB      0.028
ATOM    C10     CB      -0.15
ATOM     H5   HCMM       0.15
ATOM    C11     CB      -0.15
ATOM     H6   HCMM       0.15
ATOM    C12     CB      0.082
ATOM     O5     OR     -0.532
ATOM     H8   HOCC       0.45
ATOM    C13     CB      0.082
ATOM     O6     OR     -0.532
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ATOM      H9    HOCC        0.45
ATOM     C14      CB       -0.15
ATOM      H7    HCMM        0.15
BOND       C      C1
BOND       C      C5
BOND       C       O
BOND      C1      C2
BOND      C1       H
BOND      C2      C3
BOND      C2      O1
BOND      C3      C4
BOND      C3      C6
BOND      C4      C5
BOND      C4      O2
BOND      C5      H1
BOND       O      H2
BOND      O1      H3
BOND      C6      C7
BOND      C6      O3
BOND      C7      C8
BOND      C7      O4
BOND      C8      O2
BOND      C8      C9
BOND      O4      H4
BOND      C9     C10
BOND      C9     C14
BOND     C10     C11
BOND     C10      H5
BOND     C11     C12
BOND     C11      H6
BOND     C12     C13
BOND     C12      O5
BOND     C13     C14
BOND     C13      O6
BOND     C14      H7
BOND      O5      H8
BOND      O6      H9
ANGL       C      C1      C2
ANGL       C      C1       H
ANGL       C      C5      C4
ANGL       C      C5      H1
ANGL       C       O      H2
ANGL      C1       C      C5
ANGL      C1       C       O
ANGL      C1      C2      C3
ANGL      C1      C2      O1
ANGL     C10     C11     C12
ANGL     C10     C11      H6
ANGL     C10      C9     C14
ANGL     C10      C9      C8
ANGL     C11     C10      C9
ANGL     C11     C10      H5
ANGL     C11     C12     C13
ANGL     C11     C12      O5
ANGL     C12     C11      H6
ANGL     C12     C13     C14
ANGL     C12     C13      O6
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ANGL    C12     O5     H8
ANGL    C13    C12     O5
ANGL    C13    C14     C9
ANGL    C13    C14     H7
ANGL    C13     O6     H9
ANGL    C14    C13     O6
ANGL    C14     C9     C8
ANGL     C2     C1      H
ANGL     C2     C3     C4
ANGL     C2     C3     C6
ANGL     C2     O1     H3
ANGL     C3     C2     O1
ANGL     C3     C4     C5
ANGL     C3     C4     O2
ANGL     C3     C6     C7
ANGL     C3     C6     O3
ANGL     C4     C3     C6
ANGL     C4     C5     H1
ANGL     C4     O2     C8
ANGL     C5      C      O
ANGL     C5     C4     O2
ANGL     C6     C7     C8
ANGL     C6     C7     O4
ANGL     C7     C6     O3
ANGL     C7     C8     C9
ANGL     C7     C8     O2
ANGL     C7     O4     H4
ANGL     C8     C7     O4
ANGL     C9    C10     H5
ANGL     C9    C14     H7
ANGL     C9     C8     O2
DIHE      C      C1     C2     C3
DIHE      C      C1     C2     O1
DIHE      C      C5     C4     C3
DIHE      C      C5     C4     O2
DIHE     C1      C      C5     C4
DIHE     C1      C      C5     H1
DIHE     C1      C      O      H2
DIHE     C1     C2     C3     C4
DIHE     C1     C2     C3     C6
DIHE     C1     C2     O1     H3
DIHE    C10    C11    C12    C13
DIHE    C10    C11    C12     O5
DIHE    C10     C9    C14    C13
DIHE    C10     C9    C14     H7
DIHE    C10     C9     C8     C7
DIHE    C10     C9     C8     O2
DIHE    C11    C10     C9    C14
DIHE    C11    C10     C9     C8
DIHE    C11    C12    C13    C14
DIHE    C11    C12    C13     O6
DIHE    C11    C12     O5     H8
DIHE    C12    C11    C10     C9
DIHE    C12    C11    C10     H5
DIHE    C12    C13    C14     C9
DIHE    C12    C13    C14     H7
DIHE    C12    C13     O6     H9
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DIHE    C13     C12     C11      H6
DIHE    C13     C12      O5      H8
DIHE    C13     C14      C9      C8
DIHE    C14     C13     C12      O5
DIHE    C14     C13      O6      H9
DIHE    C14      C9     C10      H5
DIHE    C14      C9      C8      C7
DIHE    C14      C9      C8      O2
DIHE     C2      C1       C      C5
DIHE     C2      C1       C       O
DIHE     C2      C3      C4      C5
DIHE     C2      C3      C4      O2
DIHE     C2      C3      C6      C7
DIHE     C2      C3      C6      O3
DIHE     C3      C2      C1       H
DIHE     C3      C2      O1      H3
DIHE     C3      C4      C5      H1
DIHE     C3      C4      O2      C8
DIHE     C3      C6      C7      C8
DIHE     C3      C6      C7      O4
DIHE     C4      C3      C2      O1
DIHE     C4      C3      C6      C7
DIHE     C4      C3      C6      O3
DIHE     C4      C5       C       O
DIHE     C4      O2      C8      C7
DIHE     C4      O2      C8      C9
DIHE     C5       C      C1       H
DIHE     C5       C       O      H2
DIHE     C5      C4      C3      C6
DIHE     C5      C4      O2      C8
DIHE     C6      C3      C2      O1
DIHE     C6      C3      C4      O2
DIHE     C6      C7      C8      C9
DIHE     C6      C7      C8      O2
DIHE     C6      C7      O4      H4
DIHE     C8      C7      C6      O3
DIHE     C8      C7      O4      H4
DIHE     C8      C9     C10      H5
DIHE     C8      C9     C14      H7
DIHE     C9     C10     C11      H6
DIHE     C9     C14     C13      O6
DIHE     C9      C8      C7      O4
DIHE      H      C1       C       O
DIHE      H      C1      C2      O1
DIHE     H1      C5       C       O
DIHE     H1      C5      C4      O2
DIHE     H5     C10     C11      H6
DIHE     H6     C11     C12      O5
DIHE     H7     C14     C13      O6
DIHE     O2      C8      C7      O4
DIHE     O3      C6      C7      O4
DIHE     O5     C12     C13      O6
IMPR      C      C1      C5       O
IMPR     C1      C2       C       H
IMPR     C2      C3      C1      O1
IMPR     C3      C4      C2      C6
IMPR     C6      C7      C3      O3
```

```
IMPR      C7      C8      C6      O4
IMPR      C8      C9      C7      O2
IMPR      C9     C14      C8     C10
IMPR     C10     C11      C9      H5
IMPR     C11     C12     C10      H6
IMPR     C12     C13     C11      O5
IMPR     C13     C14     C12      O6
IMPR      C5      C4       C      H1
IMPR     C14     C13      C9      H7
PATCHING FIRST NONE LAST NONE
END

READ PARA CARD FLEX
*.....................................................
*. Force field parameters of the solutes
*.....................................................
*

ATOMS
MASS  101 C5A        12.011
MASS  102 C5B        12.011
MASS  103 C=C        12.011
MASS  104 C=O        12.011
MASS  105 CB         12.011
MASS  106 CR         12.011
MASS  107 HCMM        1.008
MASS  108 HOCC        1.008
MASS  109 HOCO        1.008
MASS  110 N5B        14.007
MASS  111 NC=O       14.007
MASS  112 NPYL       14.007
MASS  113 O=C        15.999
MASS  114 OR         15.999

BONDS
!
! U_bond = k ( r - r0 )^2
!
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!TYPE1    TYPE2    k [kcal/mol Angstroem^2]     r0 [Angstroem]
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
C5A       C5B                512.2560              1.3770
C5A       C=O                393.5110              1.4230
C5A       HCMM               398.0450              1.0800
C5A       N5B                599.1910              1.3130
C5A       NPYL               453.4590              1.3640
C5B       N5B                320.6820              1.3690
C5B       NC=O               428.3430              1.3760
C=C       C=C                684.0390              1.3330
C=C       C=O                328.5260              1.4680
C=C       CB                 360.3350              1.4490
C=C       OR                 397.2540              1.3730
C=O       CB                 322.9850              1.4570
C=O       NC=O               419.4910              1.3690
C=O       O=C                931.9630              1.2220
C=O       OR                 417.4760              1.3550
CB        CB                 401.0680              1.3740
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```
CB         HCMM               381.8530               1.0840
CB         OR                 404.0190               1.3760
CR         HCMM               342.9910               1.0930
CR         NC=O               335.6510               1.4360
CR         NPYL               440.0020               1.4450
HOCC       OR                 564.1430               0.9730
HOCO       OR                 532.7660               0.9810

ANGLES
!
! U_angle = k ( theta - theta0 )^2
!
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!TYPE1     TYPE2      TYPE3      k [kcal/mol rad^2]      theta0 [deg]
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
C5A        C5B        N5B              74.7000             111.6000
C5A        C5B        NC=O             67.4320             123.7000
C5A        C=O        NC=O             77.3630             114.6000
C5A        C=O        O=C              74.5560             126.5000
C5A        N5B        C5B              86.7910             103.8000
C5A        NPYL       C5A              82.9040             109.6000
C5A        NPYL       CR               61.4590             123.4000
C5B        C5A        C=O              55.1260             130.1000
C5B        C5A        NPYL             58.5080             107.3000
C5B        NC=O       C=O              75.4200             117.6000
C5B        NC=O       CR               69.0870             121.3000
C=C        C=C        C=O              39.2210             111.3000
C=C        C=C        CB               43.0350             117.5000
C=C        C=C        OR               80.3860             121.3000
C=C        C=O        CB               70.0230             112.9000
C=C        C=O        O=C              67.3600             122.6000
C=C        CB         CB               51.2400             119.7000
C=C        OR         CB              102.0470             110.7000
C=C        OR         HOCC             58.7240             105.7000
C=O        C5A        NPYL             64.7690             125.4000
C=O        C=C        OR               82.1850             116.7000
C=O        CB         CB               57.4290             114.5000
C=O        NC=O       C=O              51.0240             120.3000
C=O        NC=O       CR               59.0840             119.6000
C=O        OR         HOCO             41.9560             111.9000
CB         C=C        OR               86.2150             114.4000
CB         C=O        O=C              52.8230             120.0000
CB         C=O        OR               58.1480             102.9000
CB         CB         CB               48.1450             120.0000
CB         CB         HCMM             40.5170             120.6000
CB         CB         OR               69.6630             116.5000
CB         OR         HOCC             52.2470             105.4000
HCMM       C5A        N5B              46.2740             125.1000
HCMM       C5A        NPYL             44.4030             121.1000
HCMM       CR         HCMM             37.1340             108.8000
HCMM       CR         NC=O             53.2550             107.6000
HCMM       CR         NPYL             58.3640             106.3000
N5B        C5A        NPYL             72.8290             110.9000
N5B        C5B        NC=O             76.6430             121.1000
NC=O       C=O        NC=O            116.0090             114.9000
NC=O       C=O        O=C              65.2730             127.2000
O=C        C=O        OR               83.1200             124.4000
```

```
DIHEDRALS
!
! U_dihedral = k ( 1 + Cos[n phi - delta] )
!
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!TYPE1    TYPE2     TYPE3     TYPE4    k [kcal/mol]    n     delta [deg]
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
C5A       C5B       N5B       C5A          3.5000     2      180.0000
C5A       C5B       NC=O      C=O          3.0000     2      180.0000
C5A       C5B       NC=O      CR           3.0000     2      180.0000
C5A       C=O       NC=O      C=O          3.0000     2      180.0000
C5A       C=O       NC=O      CR           3.0000     2      180.0000
C5A       N5B       C5B       NC=O         3.5000     2      180.0000
C5A       NPYL      C5A       C5B          2.0000     2      180.0000
C5A       NPYL      C5A       C=O          2.0000     2      180.0000
C5A       NPYL      C5A       HCMM         2.0000     2      180.0000
C5A       NPYL      C5A       N5B          2.0000     2      180.0000
C5A       NPYL      CR        HCMM        -0.0570     3        0.0000
C5B       C5A       C=O       NC=O         1.2500     2      180.0000
C5B       C5A       C=O       O=C          1.2500     2      180.0000
C5B       C5A       NPYL      CR           2.0000     2      180.0000
C5B       N5B       C5A       HCMM         3.5000     2      180.0000
C5B       N5B       C5A       NPYL         3.5000     2      180.0000
C5B       NC=O      C=O       NC=O         3.0000     2      180.0000
C5B       NC=O      C=O       O=C          3.0000     2      180.0000
C5B       NC=O      CR        HCMM         0.1500     3        0.0000
C=C       C=C       C=O       CB           1.2500     2      180.0000
C=C       C=C       C=O       O=C          1.2500     2      180.0000
C=C       C=C       CB        CB           0.2170     3        0.0000
C=C       C=C       CB        CB           0.7710     2      180.0000
C=C       C=C       OR        CB           1.5500     2      180.0000
C=C       C=C       OR        HOCC         1.4050     2      180.0000
C=C       C=C       OR        HOCC        -0.1070     1        0.0000
C=C       C=C       OR        HOCC        -0.2280     3        0.0000
C=C       C=O       CB        CB           1.2500     2      180.0000
C=C       CB        CB        CB           1.0000     2      180.0000
C=C       CB        CB        HCMM         1.0000     2      180.0000
C=C       OR        CB        CB           1.6000     2      180.0000
C=O       C5A       C5B       N5B          3.5000     2      180.0000
C=O       C5A       C5B       NC=O         0.0000     1        0.0000
C=O       C5A       NPYL      CR           3.0000     2      180.0000
C=O       C=C       C=C       CB           0.9000     2      180.0000
C=O       C=C       C=C       OR           0.9000     2      180.0000
C=O       C=C       OR        HOCC         1.8000     2      180.0000
C=O       CB        CB        CB           3.5000     2      180.0000
C=O       CB        CB        HCMM         1.0000     2      180.0000
C=O       CB        CB        OR           1.0000     2      180.0000
C=O       NC=O      C5B       N5B          3.0000     2      180.0000
C=O       NC=O      C=O       NC=O         3.0000     2      180.0000
C=O       NC=O      C=O       O=C          0.3880     1        0.0000
C=O       NC=O      C=O       O=C         -0.0720     3        0.0000
C=O       NC=O      C=O       O=C         -0.2920     2      180.0000
C=O       NC=O      CR        HCMM         0.0110     3        0.0000
C=O       NC=O      CR        HCMM         0.6810     2      180.0000
C=O       NC=O      CR        HCMM        -1.0500     1        0.0000
CB        C=C       C=C       OR           0.9000     2      180.0000
```

```
CB         C=C        OR         CB             1.5500     2       180.0000
CB         C=O        C=C        OR             1.2500     2       180.0000
CB         C=O        OR         HOCO           1.9460     2       180.0000
CB         C=O        OR         HOCO          -0.0470     3         0.0000
CB         CB         C=C        OR             1.0000     2       180.0000
CB         CB         C=O        O=C            1.1280     2       180.0000
CB         CB         C=O        OR             0.8710     2       180.0000
CB         CB         CB         CB             3.5000     2       180.0000
CB         CB         CB         HCMM           3.5000     2       180.0000
CB         CB         CB         OR             3.5000     2       180.0000
CB         CB         OR         HOCC           1.4010     2       180.0000
CR         NC=O       C5B        N5B            3.0000     2       180.0000
CR         NC=O       C=O        NC=O           3.0000     2       180.0000
CR         NC=O       C=O        O=C            3.1470     2       180.0000
CR         NC=O       C=O        O=C           -0.0730     3         0.0000
CR         NC=O       C=O        O=C           -0.1600     1         0.0000
CR         NPYL       C5A        HCMM           2.0000     2       180.0000
CR         NPYL       C5A        N5B            2.0000     2       180.0000
HCMM       CB         CB         HCMM           3.5000     2       180.0000
HCMM       CB         CB         OR             3.5000     2       180.0000
HOCO       OR         C=O        O=C            0.8310     1         0.0000
HOCO       OR         C=O        O=C            3.0760     2       180.0000
HOCO       OR         C=O        O=C           -0.0290     3         0.0000
N5B        C5B        C5A        NPYL           3.5000     2       180.0000
NC=O       C5B        C5A        NPYL           3.5000     2       180.0000
NC=O       C=O        C5A        NPYL           1.2500     2       180.0000
NPYL       C5A        C=O        O=C            1.2500     2       180.0000
O=C        C=O        C=C        OR             1.2500     2       180.0000
OR         C=C        C=C        OR             6.0000     2       180.0000
OR         CB         CB         OR             3.5000     2       180.0000

IMPROPERS
! n > 0:
! U_improper = k ( 1 + Cos[n phi - delta] )
!
! n = 0:
! U_improper = k ( phi - delta )^2
!
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~

!TYPE1     TYPE2      TYPE3      TYPE4     k [kcal/mol]     n      delta [deg]
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~

C5A        C5B        NPYL       C=O            3.5980     0.0         0.0000
C5A        N5B        NPYL       HCMM           4.8940     0.0         0.0000
C5B        C5A        N5B        NC=O           2.8790     0.0         0.0000
C=C        C=C        C=O        OR             1.4390     0.0         0.0000
C=C        CB         C=C        OR             1.4390     0.0         0.0000
C=O        C=C        CB         O=C            9.3560     0.0         0.0000
C=O        NC=O       C5A        O=C            9.3560     0.0         0.0000
C=O        NC=O       NC=O       O=C            8.1320     0.0         0.0000
C=O        OR         CB         O=C            9.1400     0.0         0.0000
CB         CB         C=C        CB             2.2310     0.0         0.0000
CB         CB         CB         C=O            1.9430     0.0         0.0000
CB         CB         CB         HCMM           1.0790     0.0         0.0000
CB         CB         CB         OR             3.4540     0.0         0.0000
CR         HCMM       NC=O       HCMM           0.0000     0.0         0.0000
```

```
CR         HCMM       NPYL       HCMM            0.0000      0.0         0.0000
NC=O       C=O        C5B        CR             -1.4390      0.0         0.0000
NC=O       C=O        C=O        CR             -1.4390      0.0         0.0000
NPYL       C5A        C5A        CR              0.8640      0.0         0.0000

NONBONDED NBXMOD 5
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!TYPE1           epsilon    rmin/2       epsilon14   rmin14/2
!            [kcal/mol] [Angstroem]    [kcal/mol] [Angstroem]
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
C5A      0.00    -0.05000   2.04000
C5B      0.00    -0.05000   2.04000
C=C      0.00    -0.06800   2.09000
C=O      0.00    -0.11000   2.00000
CB       0.00    -0.07000   1.99240
CR       0.00    -0.05500   2.17500 0.00    -0.01000   2.17500
HCMM     0.00    -0.02200   1.32000
HOCC     0.00    -0.04600   0.22450
HOCO     0.00    -0.04600   0.22450
N5B      0.00    -0.20000   1.85000
NC=O     0.00    -0.20000   1.85000
NPYL     0.00    -0.09000   1.72000
O=C      0.00    -0.12000   1.70000
OR       0.00    -0.15210   1.77000
END
```

FORCE FIELD OF THE SOLVENTS

```
*============================================================
*. Force field of the solvent species
*============================================================
*

READ RTF CARD
*.............................................................
*. Topology of the solvents
*.............................................................
*
   99     1

MASS     1 H1       1.008000
MASS     2 H4       1.008000
MASS     3 H5       1.008000
MASS     4 HC       1.008000
MASS     5 HT       1.008000
MASS     6 C3      12.010000
MASS     7 CC      12.010000
MASS     8 CD      12.010000
MASS     9 CT      12.010000
MASS    10 C       12.010000
MASS    11 NA      14.010000
MASS    12 OA      16.000000
MASS    13 OT      16.000000

!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
! water
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
RESIDUE SPCE      0.000 ! spce water model, generate using noangle
   nodihedral
GROUP
ATOM OH2  OT     -0.848
ATOM H1   HT      0.424
ATOM H2   HT      0.424
BOND OH2 H1 OH2 H2 H1 H2    ! the last bond is needed for shake
ANGLE H1 OH2 H2             ! required
DONOR H1 OH2
DONOR H2 OH2
ACCEPTOR OH2
PATCHING FIRS NONE LAST NONE

!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!EMIM
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
RESIDUE EMIM  1.000
GROUP
ATOM C    C3      -0.110 !          H
ATOM H    H1       0.117 !          |
ATOM H1   H1       0.117 !      H1--C--H2
ATOM H2   H1       0.117 !          |
ATOM N    NA       0.085 !          N1
ATOM C1   CC      -0.027 !        //   \
ATOM H3   H5       0.230 !       //     C2--H4
```

```
ATOM C2   CC      -0.189 !   H3--C1     ||
ATOM H4   H4       0.253 !        \     C3--H5
ATOM N1   NA       0.085 !         \   /
ATOM C3   CD      -0.189 !           N
ATOM H5   H4       0.253 !           |
ATOM C4   C3      -0.043 !       H6--C4--H7
ATOM H6   H1       0.105 !           |
ATOM H7   H1       0.105 !       H8--C5--H9
ATOM C5   C3      -0.107 !           |
ATOM H8   HC       0.066 !           H10
ATOM H9   HC       0.066 !
ATOM H10  HC       0.066 !
BOND C     H                    ! dist      1.0796
BOND C     H1                   ! dist      1.0785
BOND C     H2                   ! dist      1.0794
BOND C     N1                   ! dist      1.4658
BOND N     C1                   ! dist      1.3138
BOND N     C3                   ! dist      1.3781
BOND N     C4                   ! dist      1.4777
BOND C1    N1                   ! dist      1.3157
BOND C1    H3                   ! dist      1.0692
BOND N1    C2                   ! dist      1.3785
BOND C2    C3                   ! dist      1.3416
BOND C2    H4                   ! dist      1.0679
BOND C3    H5                   ! dist      1.0688
BOND C4    H6                   ! dist      1.0814
BOND C4    H7                   ! dist      1.0798
BOND C4    C5                   ! dist      1.5218
BOND C5    H8                   ! dist      1.0835
BOND C5    H9                   ! dist      1.0834
BOND C5    H10                  ! dist      1.0837
ANGL C     N1    C1             ! angle   126.4111
ANGL C     N1    C2             ! angle   125.6300
ANGL H     C     H1             ! angle   109.5510
ANGL H     C     H2             ! angle   110.2559
ANGL H     C     N1             ! angle   109.2611
ANGL H1    C     H2             ! angle   109.5172
ANGL H1    C     N1             ! angle   108.8792
ANGL H2    C     N1             ! angle   109.3538
ANGL N     C1    N1             ! angle   109.8941
ANGL N     C1    H3             ! angle   125.1030
ANGL N     C3    C2             ! angle   107.1959
ANGL N     C3    H5             ! angle   122.1025
ANGL N     C4    H6             ! angle   106.7043
ANGL N     C4    H7             ! angle   106.9082
ANGL N     C4    C5             ! angle   112.0836
ANGL C1    N     C3             ! angle   107.9285
ANGL C1    N     C4             ! angle   126.1921
ANGL C1    N1    C2             ! angle   107.9577
ANGL N1    C1    H3             ! angle   125.0025
ANGL N1    C2    C3             ! angle   107.0236
ANGL N1    C2    H4             ! angle   122.0406
ANGL C2    C3    H5             ! angle   130.7003
ANGL C3    N     C4             ! angle   125.8669
ANGL C3    C2    H4             ! angle   130.9352
ANGL C4    C5    H8             ! angle   111.2780
ANGL C4    C5    H9             ! angle   111.5813
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ANGL C4    C5    H10           ! angle   109.0336
ANGL H6    C4    H7            ! angle   107.7086
ANGL H6    C4    C5            ! angle   111.3594
ANGL H7    C4    C5            ! angle   111.7864
ANGL H8    C5    H9            ! angle   108.5717
ANGL H8    C5    H10           ! angle   108.3168
ANGL H9    C5    H10           ! angle   107.9497
DIHE H     C     N1    C1      ! dihe   -120.0991
DIHE H1    C     N1    C1      ! dihe     -0.4861
DIHE H2    C     N1    C1      ! dihe    119.1407
DIHE H     C     N1    C2      ! dihe     60.3500
DIHE H1    C     N1    C2      ! dihe    179.9630
DIHE H2    C     N1    C2      ! dihe    -60.4102
DIHE C3    N     C1    N1      ! dihe     -0.0723
DIHE C4    N     C1    N1      ! dihe   -178.8479
DIHE C3    N     C1    H3      ! dihe   -179.8641
DIHE C4    N     C1    H3      ! dihe      1.3603
DIHE C1    N     C3    C2      ! dihe      0.1214
DIHE C4    N     C3    C2      ! dihe    178.9021
DIHE C1    N     C3    H5      ! dihe    179.7449
DIHE C4    N     C3    H5      ! dihe     -1.4744
DIHE C1    N     C4    H6      ! dihe    -17.3257
DIHE C3    N     C4    H6      ! dihe    164.1119
DIHE C1    N     C4    H7      ! dihe   -132.3592
DIHE C3    N     C4    H7      ! dihe     49.0783
DIHE C1    N     C4    C5      ! dihe    104.8236
DIHE C3    N     C4    C5      ! dihe    -73.7389
DIHE N     C1    N1    C       ! dihe   -179.6202
DIHE H3    C1    N1    C       ! dihe      0.1719
DIHE N     C1    N1    C2      ! dihe     -0.0039
DIHE H3    C1    N1    C2      ! dihe    179.7882
DIHE C     N1    C2    C3      ! dihe    179.7003
DIHE C1    N1    C2    C3      ! dihe      0.0802
DIHE C     N1    C2    H4      ! dihe     -0.0517
DIHE C1    N1    C2    H4      ! dihe   -179.6718
DIHE N1    C2    C3    N       ! dihe     -0.1217
DIHE H4    C2    C3    N       ! dihe    179.6001
DIHE N1    C2    C3    H5      ! dihe   -179.7009
DIHE H4    C2    C3    H5      ! dihe      0.0208
DIHE N     C4    C5    H8      ! dihe    -60.5075
DIHE H6    C4    C5    H8      ! dihe     58.9472
DIHE H7    C4    C5    H8      ! dihe    179.4809
DIHE N     C4    C5    H9      ! dihe     60.9322
DIHE H6    C4    C5    H9      ! dihe   -179.6130
DIHE H7    C4    C5    H9      ! dihe    -59.0794
DIHE N     C4    C5    H10     ! dihe   -179.9216
DIHE H6    C4    C5    H10     ! dihe    -60.4668
DIHE H7    C4    C5    H10     ! dihe     60.0669
IMPH C4    C1    N     C3
IMPH H3    N1    C1    N
IMPH C     C1    N1    C2
IMPH C3    H4    C2    N1
IMPH C2    H5    C3    N
DONOR  H3  C1
DONOR  H4  C2
DONOR  H5  C3
PATCH FIRST NONE LAST NONE
```

```
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
! acetate
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
RESIDUE OAC -1.000
GROUP
ATOM C    C3       -0.218 !     H2    O
ATOM H    HC        0.010 !     |    /
ATOM H1   HC        0.010 !  H--C---C1
ATOM H2   HC        0.010 !     |    \
ATOM C1   C         0.774 !     H1    O1
ATOM O    OA       -0.793 !
ATOM O1   OA       -0.793 !
BOND C     H                    ! dist      1.0885
BOND C     H1                   ! dist      1.0890
BOND C     H2                   ! dist      1.0858
BOND C     C1                   ! dist      1.5538
BOND C1    O                    ! dist      1.2333
BOND C1    O1                   ! dist      1.2354
ANGL C     C1    O              ! angle   116.0140
ANGL C     C1    O1             ! angle   114.5436
ANGL H     C     H1             ! angle   106.6972
ANGL H     C     H2             ! angle   109.2573
ANGL H     C     C1             ! angle   109.6829
ANGL H1    C     H2             ! angle   109.2436
ANGL H1    C     C1             ! angle   109.7254
ANGL H2    C     C1             ! angle   112.0849
ANGL O     C1    O1             ! angle   129.4425
DIHE H     C     C1    O        ! dihe   -121.4873
DIHE H1    C     C1    O        ! dihe    121.6133
DIHE H2    C     C1    O        ! dihe      0.0569
DIHE H     C     C1    O1       ! dihe     58.5127
DIHE H1    C     C1    O1       ! dihe    -58.3867
DIHE H2    C     C1    O1       ! dihe   -179.9431
IMPH C     O     C1    O1
ACCEPTOR   O  C1
ACCEPTOR  O1  C1
PATCH FIRST NONE LAST NONE
END


READ PARA CARD FLEX
*.....................................................
*. Force field parameters of the solvents
*.....................................................
*

ATOMS
MASS     1 H1       1.008000
MASS     2 H4       1.008000
MASS     3 H5       1.008000
MASS     4 HC       1.008000
MASS     5 HT       1.008000
MASS     6 C3      12.010000
MASS     7 CC      12.010000
MASS     8 CD      12.010000
MASS     9 CT      12.010000
```

```
MASS     10 C       12.010000
MASS     11 NA      14.010000
MASS     12 OA      16.000000
MASS     13 OT      16.000000

BONDS
!
! U_bond = k ( r - r0 )^2
!
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!TYPE1     TYPE2     k [kcal/mol Angstroem^2]      r0 [Angstroem]
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
HT         HT                 0.0                    1.632980862
HT         OT               450.0                    1.0000
C3         H1               335.90                   1.093
C3         NA               334.70                   1.456
CC         NA               438.80                   1.371
CD         NA               438.80                   1.371
CC         H5               356.00                   1.079
CC         CD               504.00                   1.371
CC         H4               350.10                   1.083
CD         H4               350.10                   1.083
C3         C3               303.10                   1.535
C3         HC               337.30                   1.092
C          C3               328.30                   1.508
C          OA               648.00                   1.214

ANGLES
!
! U_angle = k ( theta - theta0 )^2
!
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!TYPE1     TYPE2      TYPE3      k [kcal/mol rad^2]      theta0 [deg]
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
HT         OT         HT             55.0                  109.4667
C3         NA         CC             62.560                125.090
H1         C3         H1             39.180                109.550
H1         C3         NA             49.900                109.450
NA         CC         NA             73.650                109.330    ! SAME AS
   NA C2 NA
NA         CC         H5             49.760                122.100
NA         CD         CC             72.910                109.420
NA         CD         H4             50.220                119.660
NA         C3         C3             65.730                112.810
CC         NA         CD             63.880                128.010
CC         NA         CC             68.940                109.900
NA         CC         CD             72.910                109.420
NA         CC         H4             50.220                119.660
CC         CD         H4             47.190                129.110
CD         NA         C3             62.560                125.090
CD         CC         H4             47.190                129.110
C3         C3         HC             46.370                110.050
H1         C3         C3             46.360                110.070
HC         C3         HC             39.430                108.350
C3         C          OA             68.030                123.110
HC         C3         C              47.200                109.680
OA         C          OA             78.170                130.380
```

```
DIHEDRALS
!
! U_dihedral = k ( 1 + Cos[n phi - delta] )
!
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!TYPE1    TYPE2     TYPE3     TYPE4    k [kcal/mol]    n     delta [deg]
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
X         C3        NA        X           0.000        2       0.0
X         CC        NA        X           1.700        2     180.0
X         CD        NA        X           1.700        2     180.0
X         CC        CD        X           4.000        2     180.0
X         C3        C3        X           0.156        3       0.0
CC        NA        C3        C3          0.049        1       0.0
CC        NA        C3        C3          0.284        2     180.0
CC        NA        C3        C3          0.301        3     180.0
CC        NA        C3        C3          0.025        6       0.0
X         C         C3        X           0.000        2     180.0
HC        C3        C         OA          0.800        1       0.0
HC        C3        C         OA          0.080        3     180.0

IMPROPERS
! n > 0:
! U_improper = k ( 1 + Cos[n phi - delta] )
!
! n = 0:
! U_improper = k ( phi - delta )^2
!
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~

!TYPE1    TYPE2     TYPE3     TYPE4    k [kcal/mol]    n     delta [deg]
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~

C3        CC        NA        CD         1.100          2     180.0
H5        NA        CC        NA         1.100          2     180.0
C3        CC        NA        CC         1.100          2     180.0
CD        H4        CC        NA         1.100          2     180.0
CC        H4        CD        NA         1.100          2     180.0

NONBONDED NBXMOD 5
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!TYPE1          epsilon    rmin/2       epsilon14   rmin14/2
!           [kcal/mol] [Angstroem]    [kcal/mol] [Angstroem]
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
HT      0.00    -0.0000    0.0000
OT      0.00    -0.15210   1.7770
C3      0.00    -0.1094    1.9080      0.00    -0.0547    1.9080
H1      0.00    -0.0157    1.3870      0.00    -0.00775   1.3870
NA      0.00    -0.1700    1.8240      0.00    -0.0850    1.8240
CC      0.00    -0.0860    1.9080      0.00    -0.0430    1.9080
CD      0.00    -0.0860    1.9080      0.00    -0.0430    1.9080
H5      0.00    -0.0150    1.3590      0.00    -0.0075    1.3590
H4      0.00    -0.0150    1.4090      0.00    -0.0075    1.4090
HC      0.00    -0.0157    1.4870      0.00    -0.00775   1.4870
C       0.00    -0.0860    1.9080      0.00    -0.0430    1.9080
OA      0.00    -0.2100    1.6612      0.00    -0.1050    1.6612
END
```

HYDROGEN BONDS AND EXTRACTION YIELDS

		HBONDS		extraction yield
	c_{IL} [% wt]	water	C_2mim^+	OAc^-	[%]
caffeine					
	0	3.1±1.0			0.219±0.019
	10				0.167±0.013
	18	2.7±1.0	0.0±0.1	0.0±0.1	
	25				0.171±0.026
	36	2.3±1.0	0.0±0.1	0.0±0.1	
	40				0.204±0.010
	70	0.8±0.8	0.1±0.2	0.0±0.2	
	75				0.214±0.026
	90				0.151±0.005
	100		0.1±0.3	0.1±0.3	0.046±0.007
gallic acid					
	0	6.5±1.5			0.261±0.043
	10				0.192±0.014
	18	5.4±1.5	0.0±0.1	0.4±0.6	
	25				0.200±0.021
	36	4.6±1.4	0.0±0.2	0.9±0.6	
	40				0.190±0.029
	70	1.7±1.1	0.1±0.2	3.5±0.8	
	75				0.194±0.010
	90				0.053±0.005
	100		0.2±0.5	3.9±0.5	0.046±0.000
quercetin					
	0	7.9±1.7			0.141±0.026
	10				0.177±0.008
	18	6.5±1.7	0.0±0.2	0.5±0.6	
	25				0.183±0.010
	36	5.4±1.6	0.1±0.2	1.1±0.8	
	40				0.181±0.014
	70	2.1±1.2	0.1±0.4	3.4±0.8	
	75				0.188±0.020
	90				0.179±0.013
	100		0.2±0.4	4.7±0.6	0.142±0.005