The Porogen Effect on the Complexation Step of Trinitrotoluene-Methacrylic Acid: Towards Efficient Imprinted Polymer Sensors

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The development of sensors capable of efficient 2,4,6-trinitrotoluene detection is evolving into an important research field due to mounting threats to public safety. Molecularly imprinted polymers are receiving intensifying attention as a potential recognition element. Currently, there is limited understanding as to how the solvent impacts the crucial complexation stage in the imprinted polymer production. Here we investigate whether solvent interactions during the complexation stage should be considered in the optimal design of such sensors. The approach adopted uses molecular dynamics to simulate the interactions, between all relevant molecules, in the pre-polymerization mixture with different porogenic solvents: pure acetonitrile, dimethyl sulfoxide, water, and binary mixtures at different compositions of the former two. Molecular dynamics provide an excellent opportunity to gain an accurate insight into the behaviour of the porogen molecules with the target molecule and functional monomers. The results showed conclusive evidence towards solvent interactions impacting the complex's quality in the studied system. A porogen mixture acetonitrile:dimethyl sulfoxide of 75:25 mol ratio is suggested for the optimal trinitrotoluene and methacrylic acid complexation.

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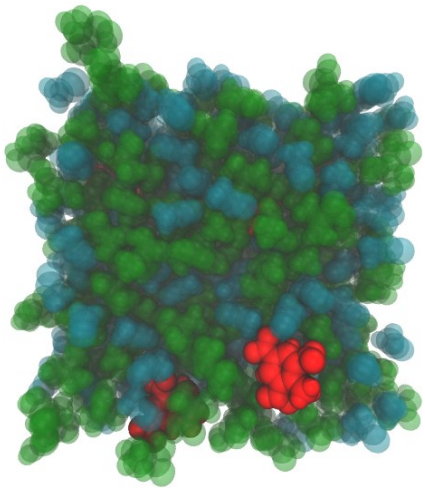
Electronic Supplementary Information (ESI): GROMACS v5.1 all topology files (.itp), quaternary NVT and NPT files (.mdp), selected final configurations files (.gro), and complete binary systems analysis are available



GROMACS *.itp files (containing all of the molecular models, including charges, bond angles etc.)

spce.itp

```
[ moleculetype ]
; molname       nrexcl
SOL             2

[ atoms ]
;   nr   type  resnr residue  atom   cgnr     charge       mass
    1  opls_116   1    SOL     OW      1     -0.8476
```

```
    2  opls_117   1    SOL    HW1      1       0.4238
    3  opls_117   1    SOL    HW2      1       0.4238

#ifndef FLEXIBLE
[ settles ]
; OW    funct   doh     dhh
1       1       0.1     0.16330

[ exclusions ]
1       2       3
2       1       3
3       1       2
#else
[ bonds ]
; i     j       funct   length  force.c.
1       2       1       0.1     345000  0.1     345000
1       3       1       0.1     345000  0.1     345000

[ angles ]
; i     j       k       funct   angle   force.c.
2       1       3       1       109.47  383     109.47  383
#endif
```

ACN.itp

```
[ moleculetype ]
; Name   nrexcl
SOL     3
[ atoms ]
;  nr  type  resnr  resid  atom  cgnr  charge    mass    total_charge
    1  opls_755  1    SOL   CA1    1   -0.514  12.0110
    2  opls_754  1    SOL   CA2    1    0.493  12.0110
    3  opls_753  1    SOL   NA3    1   -0.564  14.0067     ;  0.000
    4  opls_759  1    SOL   HA4    1    0.195   1.0080
    5  opls_759  1    SOL   HA5    1    0.195   1.0080
    6  opls_759  1    SOL   HA6    1    0.195   1.0080
; total charge of the molecule:   0.000
[ bonds ]
;  ai   aj  funct   c0         c1
    4    1    2   0.1090  1.2300e+07
    1    5    2   0.1090  1.2300e+07
    1    6    2   0.1090  1.2300e+07
    1    2    2   0.1460  4.6913e+06
    2    3    2   0.1160  4.0874e+07
[ pairs ]
;  ai   aj  funct  ;  all 1-4 pairs but the ones excluded in GROMOS itp
    4    3    1
```

```
   5    3    1
   6    3    1
[ angles ]
;  ai   aj   ak  funct   angle     fc
   4    1    5    2    108.53   443.00
   4    1    6    2    108.53   443.00
   4    1    2    2    110.30   524.00
   5    1    6    2    108.53   443.00
   5    1    2    2    110.30   524.00
   6    1    2    2    110.30   524.00
   1    2    3    2    180.00   500.00
[ dihedrals ]
; GROMOS improper dihedrals
;  ai   aj   ak   al  funct   angle     fc
[ dihedrals ]
;  ai   aj   ak   al  funct    ph0      cp     mult
[ exclusions ]
;  ai   aj  funct  ;  GROMOS 1-4 exclusions
```

DMSO.itp

```
[ moleculetype ]
; Name   nrexcl
DMSO     3
[ atoms ]
;  nr  type  resnr  resid  atom  cgnr  charge    mass    total_charge
    1 opls_004 1    DMSO    H05    1    0.159   1.0080
    2 opls_001 1    DMSO    CD2    1   -0.358  12.0110
    3 opls_004 1    DMSO    H01    1    0.159   1.0080
    4 opls_004 1    DMSO    H03    1    0.159   1.0080
    5 opls_124 1    DMSO      S    1    0.277  32.0600
    6 opls_125 1    DMSO      O    1   -0.515  15.9994     ; -0.119
    7 opls_001 1    DMSO    CD1    2   -0.358  12.0110
    8 opls_004 1    DMSO    H02    2    0.159   1.0080
    9 opls_004 1    DMSO    H04    2    0.159   1.0080
   10 opls_004 1    DMSO    H06    2    0.159   1.0080     ;  0.119
; total charge of the molecule:   0.000
[ bonds ]
;  ai   aj  funct   c0         c1
    1    2    2   0.1090   1.2300e+07
    2    3    2   0.1090   1.2300e+07
    2    4    2   0.1090   1.2300e+07
    2    5    2   0.1830   5.6200e+06
    5    6    2   0.1530   8.0400e+06
    5    7    2   0.1830   5.6200e+06
    7    8    2   0.1090   1.2300e+07
    7    9    2   0.1090   1.2300e+07
```

```
   7   10    2   0.1090   1.2300e+07
[ pairs ]
;  ai   aj  funct  ;  all 1-4 pairs but the ones excluded in GROMOS itp
   1    6    1
   1    7    1
   2    8    1
   2    9    1
   2   10    1
   3    6    1
   3    7    1
   4    6    1
   4    7    1
   6    8    1
   6    9    1
   6   10    1
[ angles ]
;  ai   aj   ak  funct   angle     fc
   1    2    3    2    109.60   450.00
   1    2    4    2    109.60   450.00
   1    2    5    2    109.60   450.00
   3    2    4    2    109.60   450.00
   3    2    5    2    109.60   450.00
   4    2    5    2    109.60   450.00
   2    5    6    2    107.00  2726.16
   2    5    7    2    100.00   475.00
   6    5    7    2    107.00  2726.16
   5    7    8    2    109.60   450.00
   5    7    9    2    109.60   450.00
   5    7   10    2    109.60   450.00
   8    7    9    2    109.60   450.00
   8    7   10    2    109.60   450.00
   9    7   10    2    109.60   450.00
[ dihedrals ]
; GROMOS improper dihedrals
;  ai   aj   ak   al  funct   angle     fc
[ dihedrals ]
;  ai   aj   ak   al  funct    ph0      cp     mult
   3    2    5    6    1    180.00     1.00    6
   6    5    7    8    1    180.00     1.00    6
[ exclusions ]
;  ai   aj  funct  ;  GROMOS 1-4 exclusions
```

MAA.itp

```
[ moleculetype ]
; Name   nrexcl
MAA     3
```

```
[ atoms ]
;  nr  type  resnr  resid  atom  cgnr  charge    mass    total_charge
    1 opls_004  1    MAA     HM8    1    0.197   1.0080
    2 opls_001  1    MAA     CM1    1   -0.459  12.0110
    3 opls_004  1    MAA     HM7    1    0.203   1.0080     ; -0.059
    4 opls_001  1    MAA     CM2    2    0.164  12.0110
    5 opls_001  1    MAA     CM4    2    0.587  12.0110
    6 opls_268  1    MAA     OM5    2   -0.552  15.9994
    7 opls_269  1    MAA     OM6    2   -0.596  15.9994
    8 opls_270  1    MAA    HM12    2    0.456   1.0080     ;  0.059
    9 opls_267  1    MAA     CM3    3   -0.354  12.0110
   10 opls_004  1    MAA     HM9    3    0.118   1.0080
   11 opls_004  1    MAA    HM10    3    0.118   1.0080
   12 opls_004  1    MAA    HM11    3    0.118   1.0080     ;  0.000
; total charge of the molecule:   0.000
[ bonds ]
;  ai   aj  funct   c0        c1
    1    2    2   0.1090   1.2300e+07
    2    3    2   0.1090   1.2300e+07
    2    4    2   0.1340   1.1700e+07
    4    5    2   0.1500   8.3700e+06
    4    9    2   0.1510   3.7279e+06
    5    6    2   0.1230   1.6600e+07
    5    7    2   0.1360   1.0200e+07
    7    8    2   0.0972   1.9581e+07
    9   10    2   0.1090   1.2300e+07
    9   11    2   0.1090   1.2300e+07
    9   12    2   0.1090   1.2300e+07
[ pairs ]
;  ai   aj  funct  ;  all 1-4 pairs but the ones excluded in GROMOS itp
    1    5    1
    1    9    1
    2    6    1
    2    7    1
    2   10    1
    2   11    1
    2   12    1
    3    5    1
    3    9    1
    4    8    1
    5   10    1
    5   11    1
    5   12    1
    6    8    1
    6    9    1
    7    9    1
[ angles ]
;  ai   aj   ak  funct   angle     fc
```

```
    1    2    3    2    119.00  2211.40
    1    2    4    2    120.00   505.00
    3    2    4    2    120.00   505.00
    2    4    5    2    120.00   560.00
    2    4    9    2    126.00   640.00
    5    4    9    2    111.00   530.00
    4    5    6    2    126.00   640.00
    4    5    7    2    115.00   610.00
    6    5    7    2    124.00   730.00
    5    7    8    2    109.50   450.00
    4    9   10    2    109.00  1680.51
    4    9   11    2    109.00  1680.51
    4    9   12    2    109.00  1680.51
   10    9   11    2    108.53   443.00
   10    9   12    2    108.53   443.00
   11    9   12    2    108.53   443.00
 [ dihedrals ]
 ; GROMOS improper dihedrals
 ;  ai   aj   ak   al  funct   angle     fc
    5    4    7    6    2      0.00   167.36
    4    5    2    9    2      0.00   167.36
    2    4    3    1    2      0.00   167.36
 [ dihedrals ]
 ;  ai   aj   ak   al  funct    ph0      cp     mult
    3    2    4    5    1    180.00    41.80    2
    2    4    5    7    1    180.00     5.86    2
    5    4    9   10    1    180.00     1.00    6
    4    5    7    8    1    180.00    16.70    2
 [ exclusions ]
 ;  ai   aj  funct  ;  GROMOS 1-4 exclusions
```

TNT.itp

```
[ atomtypes ]
; name  bond_type  mass      charge   ptype     sigma (nm)   epsilon (kJ mol-1)
 CB    C         12.011    0.000    A         0.355        0.292880
 HB    H          1.008    0.000    A         0.242        0.125520
 CT    C         12.011    0.000    A         0.350        0.276144
 HT    H          1.008    0.000    A         0.250        0.125520
 NB    N         14.007    0.000    A         0.325        0.502080
 ON    O         15.999    0.000    A         0.296        0.711280

[ moleculetype ]
; Tri Nitro Toluene
```

```
; CAS Number  Molecular Weight
; Name  nrexcl
  TNT   3

[ atoms ]
;      nr      type    resnr   residue atom    cgnr  charge
       1       CB      1       TNT     C1      1       0.090
       2       CB      1       TNT     C2      2      -0.115
       3       CB      1       TNT     C3      3       0.090
       4       CB      1       TNT     C4      4      -0.115
       5       CB      1       TNT     C5      5       0.090
       6       CB      1       TNT     C6      6      -0.115
       7       HB      1       TNT     H41     4       0.115
       8       HB      1       TNT     H61     6       0.115
       9       CT      1       TNT     C7      2      -0.065
      10       HT      1       TNT     H71     2       0.060
      11       HT      1       TNT     H72     2       0.060
      12       HT      1       TNT     H73     2       0.060
      13       NB      1       TNT     N3      3       0.650
      14       ON      1       TNT     O31     3      -0.370
      15       ON      1       TNT     O32     3      -0.370
      16       NB      1       TNT     N1      1       0.650
      17       ON      1       TNT     O11     1      -0.370
      18       ON      1       TNT     O12     1      -0.370
      19       NB      1       TNT     N5      5       0.650

      20       ON      1       TNT     O51     5      -0.370
      21       ON      1       TNT     O52     5      -0.370

[ bonds ]
; ai  aj   funct   c0      c1
  1   2      1     0.1400  392721.8
  1   6      1     0.1400  392721.8
  1  16      1     0.1460  334944.0
  2   3      1     0.1400  392721.8
  2   9      1     0.1510  265443.1
  3   4      1     0.1400  392721.8
```

```
 3  13      1     0.1460  334944.0
 4   5      1     0.1400  392721.8
 4   7      1     0.1080  307311.1
 5   6      1     0.1400  392721.8
 5  19      1     0.1460  334944.0
 6   8      1     0.1080  307311.1
 9  10      1     0.1090  284702.4
 9  11      1     0.1090  284702.4
 9  12      1     0.1090  284702.4
13  14      1     0.1225  460548.0
13  15      1     0.1225  460548.0
16  17      1     0.1225  460548.0
16  18      1     0.1225  460548.0
19  20      1     0.1225  460548.0
19  21      1     0.1225  460548.0

[ angles ]
; ai   aj  ak  funct  c0      c1
 1    2   3     1    120.00  527.537
 1    2   9     1    120.00  586.152
 1    6   5     1    120.00  527.537
 1    6   8     1    120.00  293.076
 1   16  17     1    117.50  669.888
 1   16  18     1    117.50  669.888
 2    1   6     1    120.00  527.537
 2    1  16     1    120.00  711.756
 2    3   4     1    120.00  527.537
 2    3  13     1    120.00  711.756
 2    9  10     1    109.50  293.076
 2    9  11     1    109.50  293.076
 2    9  12     1    109.50  293.076
 3    2   9     1    120.00  586.152
 3    4   5     1    120.00  527.537
 3    4   7     1    120.00  293.076
 3   13  14     1    117.50  669.888
 3   13  15     1    117.50  669.888
 4    3  13     1    120.00  711.756
```

```
 4   5   6    1   120.00  527.537
 4   5  19    1   120.00  711.756
 5   4   7    1   120.00  293.076
 5   6   1    1   120.00  527.537
 5   6   8    1   120.00  293.076
 5  19  20    1   117.50  669.888
 5  19  21    1   117.50  669.888
 6   5  19    1   120.00  711.756
 6   1  16    1   120.00  711.756
10   9  11    1   107.80  276.329
10   9  12    1   107.80  276.329
11   9  12    1   107.80  276.329
14  13  15    1   125.00  669.888
17  16  18    1   125.00  669.888
20  19  21    1   125.00  669.888
[ dihedrals ]
; Propers
;  C*    CT    CT    HC    3     0.96715   2.90145   0.00000  -3.86860   0.00000   0.00000 ; aromatics
; ai  aj  ak  al funct  c0       c1       c2       c3       c4       c5
 1   6   5   19 3     0.96715   2.90145   0.00000  -3.86860   0.00000   0.00000
 1   2   3   13 3     0.96715   2.90145   0.00000  -3.86860   0.00000   0.00000
 2   1   6   8  3     0.96715   2.90145   0.00000  -3.86860   0.00000   0.00000
 2   3   4   7  3     0.96715   2.90145   0.00000  -3.86860   0.00000   0.00000
 3   2   1   16 3     0.96715   2.90145   0.00000  -3.86860   0.00000   0.00000
 3   4   5   19 3     0.96715   2.90145   0.00000  -3.86860   0.00000   0.00000
 4   3   2   9  3     0.96715   2.90145   0.00000  -3.86860   0.00000   0.00000
 4   5   6   8  3     0.96715   2.90145   0.00000  -3.86860   0.00000   0.00000
 5   4   3   13 3     0.96715   2.90145   0.00000  -3.86860   0.00000   0.00000
 5   6   1   16 3     0.96715   2.90145   0.00000  -3.86860   0.00000   0.00000
 6   1   2   9  3     0.96715   2.90145   0.00000  -3.86860   0.00000   0.00000
 6   5   4   7  3     0.96715   2.90145   0.00000  -3.86860   0.00000   0.00000
 7   4   5   19 3     0.96715   2.90145   0.00000  -3.86860   0.00000   0.00000
 19  5   6   8  3     0.96715   2.90145   0.00000  -3.86860   0.00000   0.00000
 8   6   1   16 3     0.96715   2.90145   0.00000  -3.86860   0.00000   0.00000
 16  1   2   9  3     0.96715   2.90145   0.00000  -3.86860   0.00000   0.00000
 9   2   3   13 3     0.96715   2.90145   0.00000  -3.86860   0.00000   0.00000
 13  3   4   7  3     0.96715   2.90145   0.00000  -3.86860   0.00000   0.00000
```

;nitrobenzene

; CA CA NT H 3 8.49920 0.00000 -8.49920 0.00000 0.00000 0.00000 ; aniline

; ai aj ak al funct c0 c1 c2 c3 c4 c5

2 3 13 14 3 8.49920 0.00000 -8.49920 0.00000 0.00000 0.00000

2 3 13 15 3 8.49920 0.00000 -8.49920 0.00000 0.00000 0.00000

4 3 13 14 3 8.49920 0.00000 -8.49920 0.00000 0.00000 0.00000

4 3 13 15 3 8.49920 0.00000 -8.49920 0.00000 0.00000 0.00000

2 1 16 17 3 8.49920 0.00000 -8.49920 0.00000 0.00000 0.00000

2 1 16 18 3 8.49920 0.00000 -8.49920 0.00000 0.00000 0.00000

6 1 16 17 3 8.49920 0.00000 -8.49920 0.00000 0.00000 0.00000

6 1 16 18 3 8.49920 0.00000 -8.49920 0.00000 0.00000 0.00000

4 5 19 20 3 8.49920 0.00000 -8.49920 0.00000 0.00000 0.00000

4 5 19 21 3 8.49920 0.00000 -8.49920 0.00000 0.00000 0.00000

6 5 19 20 3 8.49920 0.00000 -8.49920 0.00000 0.00000 0.00000

6 5 19 21 3 8.49920 0.00000 -8.49920 0.00000 0.00000 0.00000

; Improper OPLS dihedrals

; ai aj ak al funct angle ka n

1 2 3 4 1 180.0 4.60548 2

2 3 4 5 1 180.0 4.60548 2

3 4 5 6 1 180.0 4.60548 2

4 5 6 1 1 180.0 4.60548 2

5 6 1 2 1 180.0 4.60548 2

6 1 2 3 1 180.0 4.60548 2

; the followings are to keep the meythyl group in the same plane as the aromatic ring

2 1 3 9 1 180.0 100 2

2 6 4 9 1 180.0 100 2

5 1 3 9 1 180.0 100 2

5 6 4 9 1 180.0 100 2

16 1 2 9 1 180.0 100 2

13 3 2 9 1 180.0 100 2

[pairs]

;excluding the 1-4 for OPLS the atoms 3 bonds appart

; ai al funct co c1

1 4 1 0.000 0.000

1 10 1 0.000 0.000

1 11 1 0.000 0.000

1 12 1 0.000 0.000

1 19 1 0.000 0.000

2 5 1 0.000 0.000

2 17 1 0.000 0.000

2 18 1 0.000 0.000

2 14 1 0.000 0.000

2 15 1 0.000 0.000

2 7 1 0.000 0.000

2 8 1 0.000 0.000

3 10 1 0.000 0.000

3 11 1 0.000 0.000

3 12 1 0.000 0.000

3 16 1 0.000 0.000

3 6 1 0.000 0.000

3 19 1 0.000 0.000

4 9 1 0.000 0.000

4 8 1 0.000 0.000

5 16 1 0.000 0.000

5 13 1 0.000 0.000

6 17 1 0.000 0.000

6 18 1 0.000 0.000

6 9 1 0.000 0.000

6 20 1 0.000 0.000

6 21 1 0.000 0.000

6 7 1 0.000 0.000

7 19 1 0.000 0.000

7 13 1 0.000 0.000

8 19 1 0.000 0.000

8 16 1 0.000 0.000

9 16 1 0.000 0.000

9 13 1 0.000 0.000

9 14 1 0.000 0.000

9 15 1 0.000 0.000

9 17 1 0.000 0.000

9 18 1 0.000 0.000

10 13 1 0.000 0.000

10 14 1 0.000 0.000

10 15 1 0.000 0.000

10 16 1 0.000 0.000

10 17 1 0.000 0.000

10 18 1 0.000 0.000

11 13 1 0.000 0.000

11 14 1 0.000 0.000

11 15 1 0.000 0.000

11 16 1 0.000 0.000

11 17 1 0.000 0.000

11 18 1 0.000 0.000

12 13 1 0.000 0.000

12 14 1 0.000 0.000

12 15 1 0.000 0.000

12 16 1 0.000 0.000

12 17 1 0.000 0.000

12 18 1 0.000 0.000

GROMACS quaternary .mdp files.

NPT.mdp

constraints = all-bonds

unconstrained-start=no

integrator = md

dt = 0.0002

tinit = 0.0

nsteps = 4000000

nstcomm = 1000

nstxout = 50000

nstvout = 50000

nstxtcout = 250

xtc_precision = 1000

nstfout = 0

nstlog = 10000

nstenergy = 1000

nstlist = 5

ns_type = grid

coulombtype = pme

cutoff-scheme = Verlet

rlist = 1.0

rcoulomb = 1.0

rvdw = 1.0

fourierspacing = 0.15

pme_order = 6

ewald_rtol = 1.E-5

optimize_fft = yes

; Nose-hoover thermostat is ON for both groups

Tcoupl = berendsen

tc-grps = TNT MAA ACN DMSO

tau_t = 0.2 0.2 0.2 0.2

ref_t = 298.15 298.15 298.15 298.15

; Energy monitoring

energygrps =

; Isotropic pressure coupling is now off

Pcoupl = berendsen

Pcoupltype = isotropic

tau_p = 1.0

compressibility = 4.5e-5

ref_p = 1.0

; Generate velocites is on at 300 K.

gen_vel = no

gen_temp = 298.15

gen_seed = 89713

pbc = xyz

;Have a nice simulation!

NVT.mdp

constraints = all-bonds

unconstrained-start=no

integrator = md

dt = 0.002

tinit = 0.0

nsteps = 1000000

nstcomm = 1000

nstxout = 50000

nstvout = 50000

nstxtcout = 250

xtc_precision = 1000

nstfout = 0

nstlog = 10000

nstenergy = 1000

nstlist = 5

ns_type = grid

coulombtype = pme

cutoff-scheme = Verlet

rlist = 1.0

rcoulomb = 1.0

rvdw = 1.0

fourierspacing = 0.15

pme_order = 6

ewald_rtol = 1.E-5

optimize_fft = yes

; Nose-hoover thermostat is ON for both groups

Tcoupl = nose-hoover

tc-grps = TNT MAA ACN DMSO

tau_t = 0.2 0.2 0.2 0.2

ref_t = 298.15 298.15 298.15 298.15

; Energy monitoring

energygrps =

; Isotropic pressure coupling is now off

Pcoupl = no

Pcoupltype = isotropic

tau_p = 1.0

compressibility = 4.5e-5

ref_p = 1.0

; Generate velocites is on at 300 K.

gen_vel = no

gen_temp = 298.15

gen_seed = 89713

pbc = xyz

;Have a nice simulation!

GROMACS selected final configurations .gro files.

- boxTNTMAAACN.gro
- boxTNTMAADMSO.gro
- boxTNTMAAWater.gro
- boxTNTMAAACNDMSO75.25.gro

Two-Component Systems

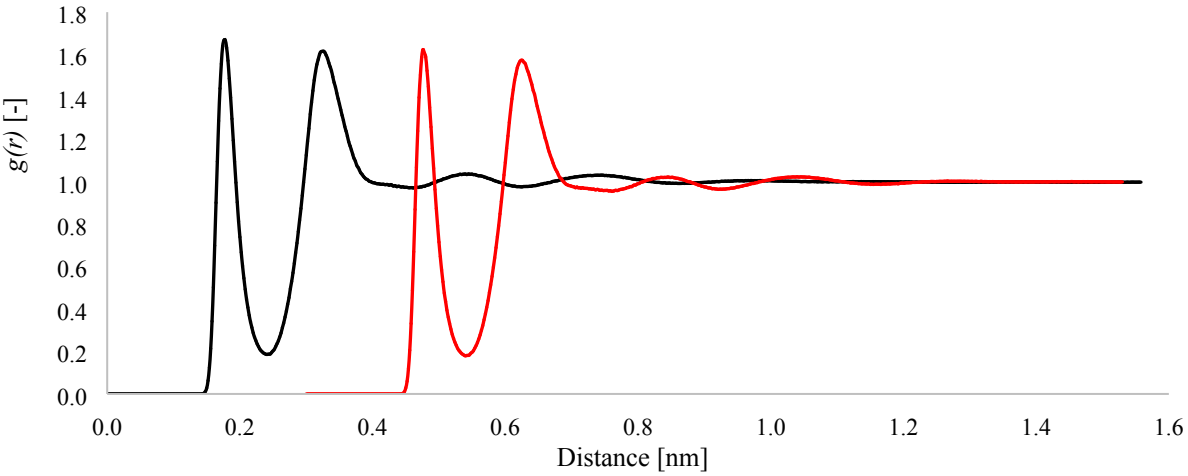


Figure A. Water-Water RDF in TNT:water (black) and the pure water (red) systems.

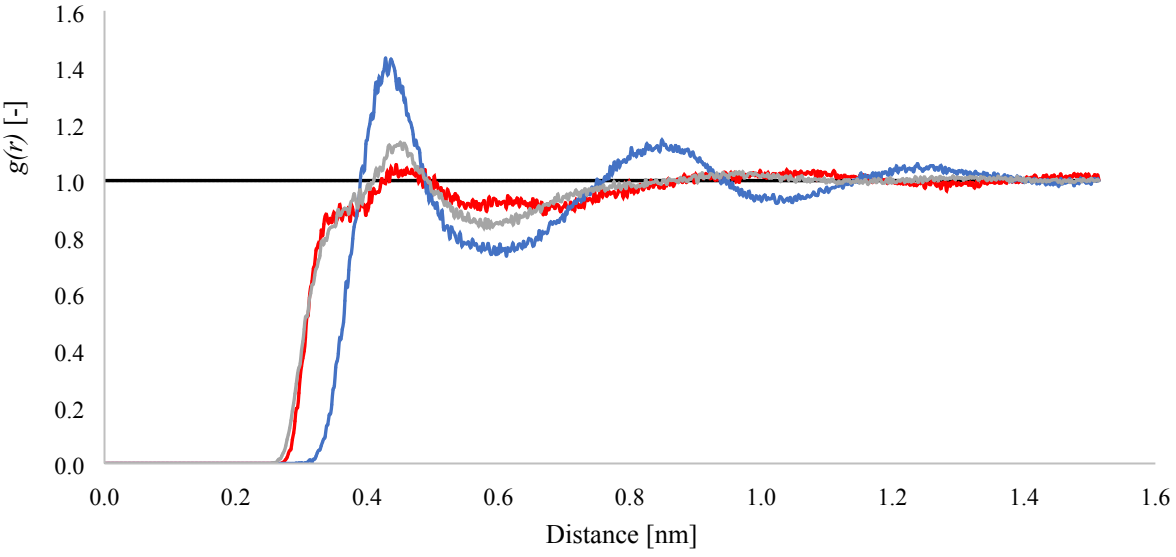


Figure B. RDFs analysis between ACN and TNT atoms, N_{ACN}-N_{TNT} (red), $CH_{3\,ACN}$-N_{TNT} (blue) and C_{ACN}-O_{TNT} (grey).

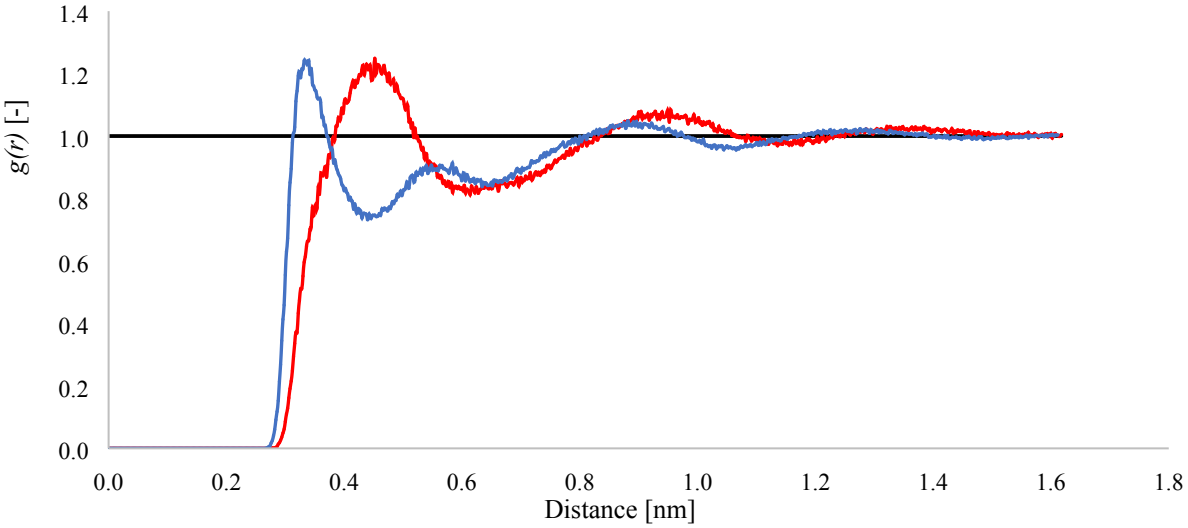


Figure C. RDFs analysis between DMSO and TNT atoms, S_{DMSO}-O_{TNT} (red), $CH_{3\ DMSO}$-O_{TNT} (blue)

Table A. TNT-ACN and TNT-DMSO KBI and maximum points.

Porogen	Kirkwood-Buff Integral $[nm^3]$	Maximum Point [-]
CAN	0.0594	1.51
DMSO	0.0121	1.24

Table B TNT-ACN and TNT-DMSO maximum and average cluster sizes around the TNT oxygen atoms.

Solvent	Maximum Cluster Size [-]	Average Cluster Size [-]
ACN	22	2.28
DMSO	10	2.15

Three-Component Systems

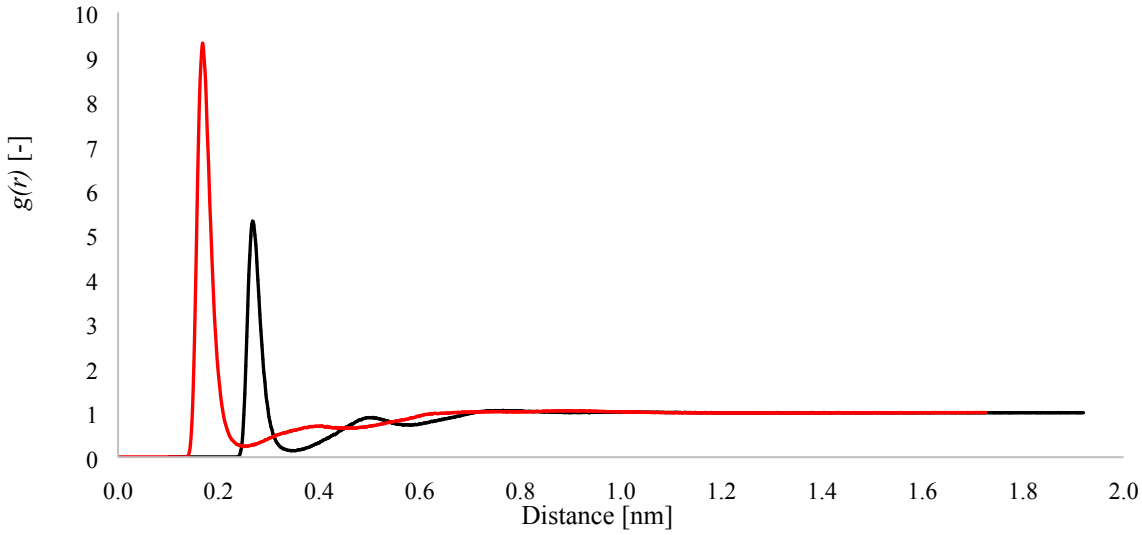


Figure D MAA-MAA RDFs in the TNT:MAA (red) and TNT:MAA:water (black, shifted 0.1 nm in x) systems.

Table C MAA maximum and average cluster sizes for various systems.

System	Maximum Cluster Size [-]	Average Cluster Size [-]
Pure MAA	28	4.51
TNT:MAA	26	4.41
TNT:MAA:Water	16	3.21
TNT:MAA:ACN	13	3.19
TNT:MAA:DMSO	07	2.58

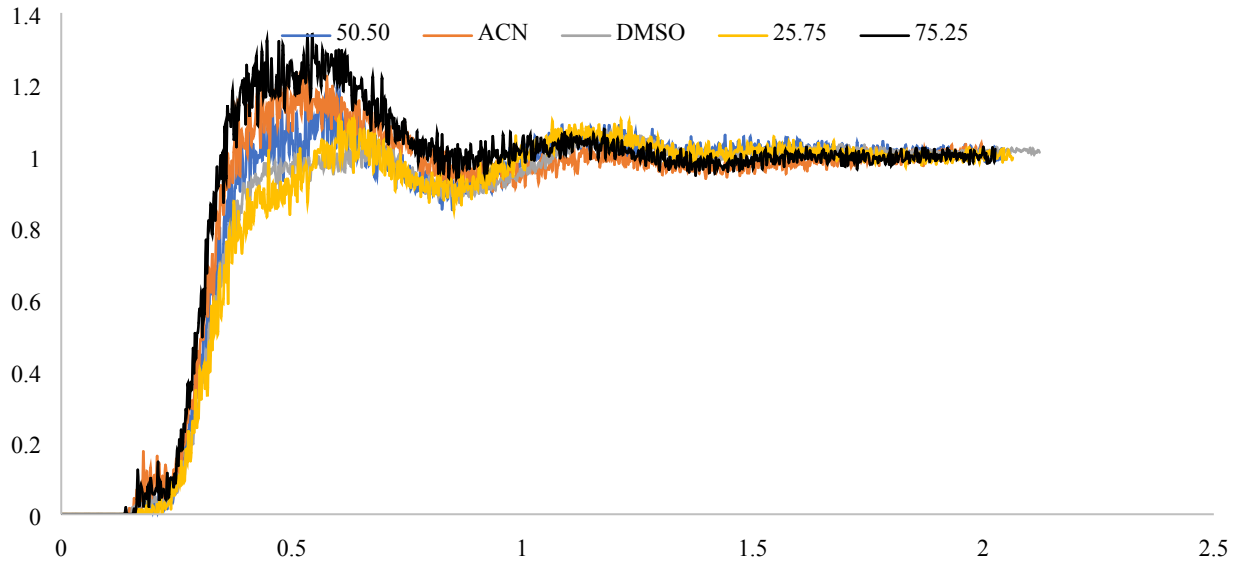


Figure E. MAA-MAA RDFs for the binary porogen ACN:DMSO.