ESI for: On the coordination of Zn^{2+} ion in Tf_2N^- based Ionic Liquids: Structural and dynamic properties at varying nature of the organic cation.

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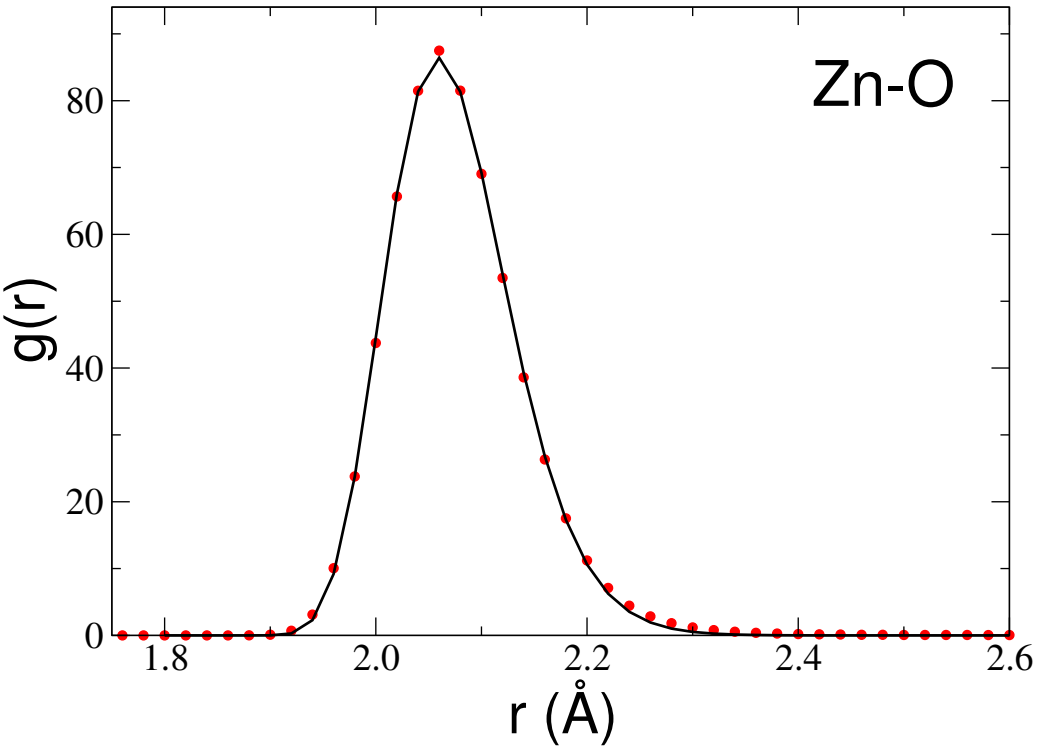

Figure S1. Zn-O $g(r)$ obtained from the MD simulation of $Zn(Tf_2N)_2$ solution in the $[C_8(mim)_2](Tf_2N)_2$ IL (dotted red line) and corresponding Gamma-like peak obtained from the fitting procedure (solid black line).

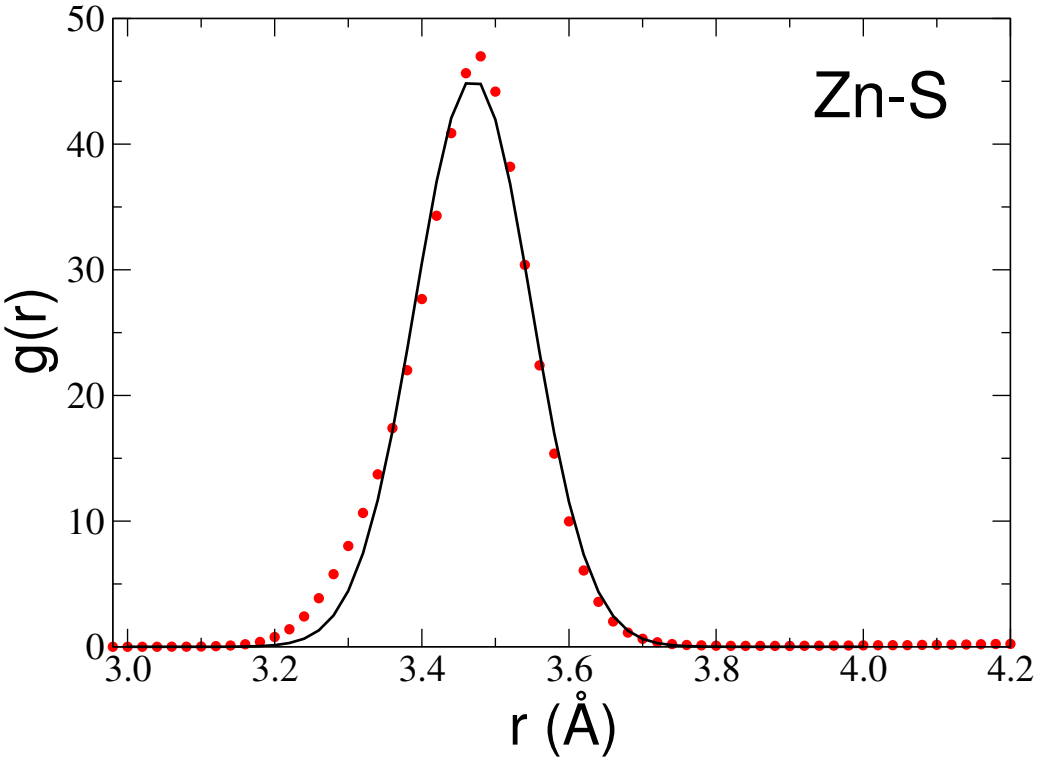

Figure S2. Zn-S $g(r)$ obtained from the MD simulation of $Zn(Tf_2N)_2$ solution in the $[C_8(mim)_2](Tf_2N)_2$ IL (dotted red line) and corresponding Gamma-like peak obtained from the fitting procedure (solid black line).

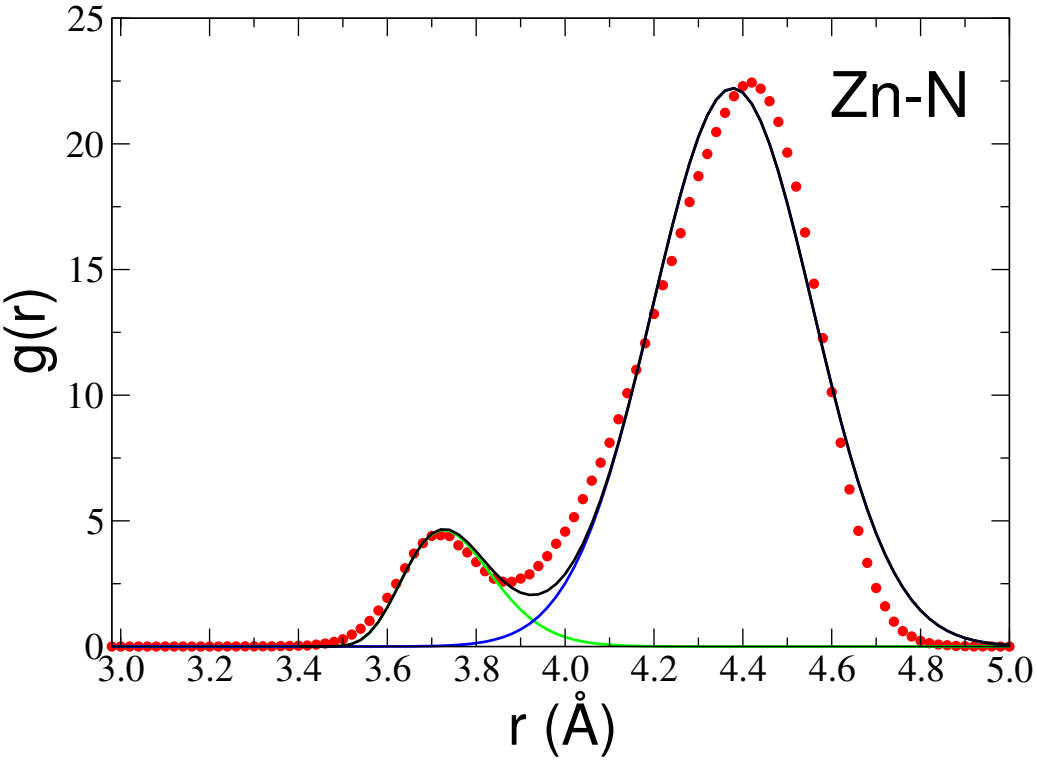

Figure S3. Zn-N $g(r)$ obtained from the MD simulation of $Zn(Tf_2N)_2$ solution in the $[C_8(mim)_2](Tf_2N)_2$ IL (dotted red line) and corresponding Gamma-like Zn-N_1 (solid green line) and Zn-N_2 (solid blue line) peaks together with their sum (solid black line) obtained from the fitting procedure.

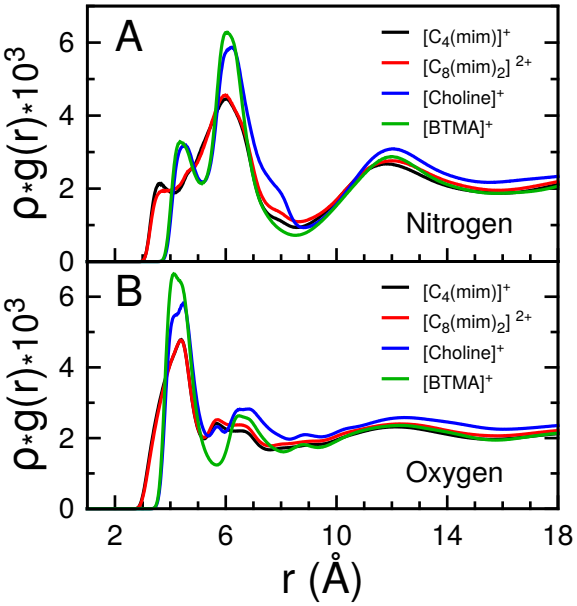

Figure S4. Cation-anion radial distribution functions multiplied by the numerical density of the observed atoms, $g(r) \cdot \rho$, calculated from the MD simulations of $Zn(Tf_2N)_2$ solutions in Tf_2N^- based ILs with different organic cations: $[C_4(mim)]^+$ (black lines), $[C_8(mim)_2]^{2+}$ (red lines), $[Choline]^+$ (blue lines) and $[BTMA]^+$ (green lines). The $g(r) \cdot \rho$'s are calculated between either the imidazolium ring geometrical centers (for $[C_4(mim)]^+$ and $[C_8(mim)_2]^{2+}$ cations) or the quaternary nitrogen atom (for $[Choline]^+$ and $[BTMA]^+$ cations) and Tf_2N^- nitrogen (A) or oxygen (B) atoms.

SDFs of the organic cation around the Tf_2N^- anion

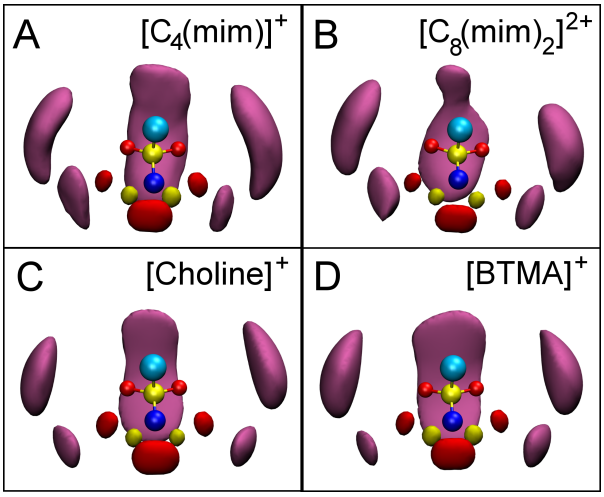

Figure S5. Spatial distribution functions (SDFs) of the organic cation (mauve surface) around the Tf_2N^- anion calculated from the MD simulations. The atoms of the anion sulfonyl group used to build the internal reference system are shown explicitly, with the trifluoromethyl substituent depicted as a cyan sphere. The other sulfonyl group is represented by intramolecular SDFs of the sulfur (yellow surface) and oxygen (red surface) atoms. The SDFs for the $[C_4(mim)]^+$ (A) and $[C_8(mim)_2]^{2+}$ (B) cations are evaluated by considering the imidazolium ring geometrical centers, while the SDFs for $[Choline]^+$ (C) and $[BTMA]^+$ (D) using the quaternary nitrogen atom.

Fig. S5 shows the spatial distribution functions (SDFs) of the different organic cations around the Tf_2N^- anion. The isodensity surfaces of the imidazolium ring geometrical centers have been calculated for $[C_4(mim)]^+$ and $[C_8(mim)_2]^{2+}$ cations, while for $[Choline]^+$ and $[BTMA]^+$ cations the quaternary nitrogen atoms have been used. This analysis has been carried out in an internal reference system integral with one of the sulfonyl groups of the Tf_2N^- anion, and, since it is known that this anion has two stable conformers, we have also computed intramolecular SDFs for the sulfur and oxygen atoms of the other sulfonyl group. The SDFs for all the IL solutions show three wide distributions of cations around the Tf_2N^- sulfonyl group. Interestingly, these distributions are not located along the S-O direction but rather are found in between two S-O directions, in such a way that the or-

ganic cations can simultaneously interact with two oxygen atoms of the anion. Moreover, in the case of the $[C_8(mim)_2]^{2+}$ cation the isosurface between the two S-O directions of the same sulfonyl group (i.e. the central one) shows a vertical asymmetry: the $[C_8(mim)_2]^{2+}$ cation is more likely to be found below the sulfonyl plane than above it. This is due to the presence above the plane of the trifluoromethyl substituent that sterically hinders the coordination of the $[C_8(mim)_2]^{2+}$ cation, as it is much bulkier than the other IL cations investigated in this work. Another common feature in the SDFs of all the cations is the presence of two smaller isosurfaces located on the opposite side with respect to the sulfonyl group used as reference system. These small spots are closer to the anion center of mass than the other isosurfaces and can be attributed to the presence of organic cations directly interacting with the nitrogen atom of the Tf_2N^- anion.

Input files for the $[C_4(mim)][Tf_2N]$ system

```
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; bistriflimide
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; dialkylimidazolium
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;;;;;;;;;;;;;;;;;;
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;;;;;;;;;;;;;;;;;;
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;4   6

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15  12  9   10  5   0.00000  0.00000   1.4510   0.00000
15  12  9   11  5   0.00000  0.00000   1.4510   0.00000
```

```
;;;;;;;;;;;;;;;;;;
; Zinc
;;;;;;;;;;;;;;;;;;
[ moleculetype ]
ZnX    3
[atoms]
;nr type    resnr   res atom    cgnr    chrg    mass
1   Zn  1   ZnX    Zn    1   2.0000   65.3900
```

$[C_4(mim)][Tf_2N]$ system topology

```
[ defaults ]
; nbfunc        comb-rule       gen-pairs       fudgeLJ fudgeQQ
  1             2               yes              0.5     0.5

#include "atomtypes.itp"
#include "zn.itp"
#include "c4mim.itp"
#include "tf2n.itp"

[ system ]
; The name of the system to be simulated
Zn_Tf2N in C4mim_Tf2N

[ molecules ]
; Molname   Number
ZnX              5
TFN            180
C4IM           170
```

Input files for the $[C_8(mim)_2][Tf_2N]_2$ system

```
[ atomtypes ]
; name      mass      charge      ptype      sigma      epsilon
; metallic cations
   Zn   65.39000       +2.000       A   1.95000e-01   1.04600e+00
; bistriflimide
   F1   18.99800      -0.1600       A   2.95000e-01   2.21750e-01
   CBT  12.01100       0.3500       A   3.50000e-01   2.76140e-01
   SBT  32.06600       1.0200       A   3.55000e-01   1.04600e+00
   OBT  15.99900      -0.5300       A   2.96000e-01   8.78640e-01
   NBT  14.00670      -0.6600       A   3.25000e-01   7.11280e-01
; dialkylimidazolium (also dicationic)
   NA   14.00670       0.1500       A   3.25000e-01   7.11280e-01
   C1   12.01100      -0.1700       A   3.50000e-01   2.76140e-01
   C2   12.01100       0.0100       A   3.50000e-01   2.76140e-01
   CS   12.01100      -0.1200       A   3.50000e-01   2.76140e-01
   CT   12.01100      -0.1800       A   3.50000e-01   2.76140e-01
   CR   12.01100      -0.1100       A   3.55000e-01   2.92880e-01
   CW   12.01100      -0.1300       A   3.55000e-01   2.92880e-01
   HCR   1.00800       0.2100       A   2.42000e-01   1.25520e-01
   HCW   1.00800       0.2100       A   2.42000e-01   1.25520e-01
   HC    1.00800       0.0600       A   2.50000e-01   1.25520e-01
   H1    1.00800       0.1300       A   2.50000e-01   1.25520e-01
```

```
;;;;;;;;;;;;;;;;;;
; 1,8-bis(3-methylimidazolium-1-yl)octane
;;;;;;;;;;;;;;;;;;
[ moleculetype ]
C8IM2    3
[atoms]
;nr type    resnr   res atom    cgnr    chrg    mass
1   HCW 1   C8IM2  HCW1  1   0.2100   1.0080
2   CW  1   C8IM2  CW1   1  -0.1300  12.0110
3   CW  1   C8IM2  CW2   1  -0.1300  12.0110
4   HCW 1   C8IM2  HCW2  1   0.2100   1.0080
5   NA  1   C8IM2  NA1   1   0.1500  14.0070
6   CR  1   C8IM2  CR1   1  -0.1100  12.0110
7   HCR 1   C8IM2  HCR1  1   0.2100   1.0080
8   NA  1   C8IM2  NA2   1   0.1500  14.0070
9   C1  1   C8IM2  C11   1  -0.1700  12.0110
10  H1  1   C8IM2  H11   1   0.1300   1.0080
11  H1  1   C8IM2  H12   1   0.1300   1.0080
12  H1  1   C8IM2  H13   1   0.1300   1.0080
13  C1  1   C8IM2  C12   1  -0.1700  12.0110
14  H1  1   C8IM2  H14   1   0.1300   1.0080
15  H1  1   C8IM2  H15   1   0.1300   1.0080
16  C2  1   C8IM2  C21   1   0.0100  12.0110
17  HC  1   C8IM2  HC1   1   0.0600   1.0080
18  HC  1   C8IM2  HC2   1   0.0600   1.0080
19  C1  1   C8IM2  C13   1  -0.1700  12.0110
20  H1  1   C8IM2  H16   1   0.1300   1.0080
21  H1  1   C8IM2  H17   1   0.1300   1.0080
22  HCW 1   C8IM2  HCW3  1   0.2100   1.0080
23  CW  1   C8IM2  CW3   1  -0.1300  12.0110
24  CW  1   C8IM2  CW4   1  -0.1300  12.0110
25  HCW 1   C8IM2  HCW4  1   0.2100   1.0080
26  NA  1   C8IM2  NA3   1   0.1500  14.0070
27  CR  1   C8IM2  CR2   1  -0.1100  12.0110
28  HCR 1   C8IM2  HCR2  1   0.2100   1.0080
29  NA  1   C8IM2  NA4   1   0.1500  14.0070
30  C1  1   C8IM2  C14   1  -0.1700  12.0110
31  H1  1   C8IM2  H18   1   0.1300   1.0080
```

```
32  H1  1   C8IM2  H19   1   0.1300   1.0080
33  H1  1   C8IM2  H110  1   0.1300   1.0080
34  CS  1   C8IM2  CS1   1  -0.1200  12.0110
35  CS  1   C8IM2  CS2   1  -0.1200  12.0110
36  CS  1   C8IM2  CS3   1  -0.1200  12.0110
37  CS  1   C8IM2  CS4   1  -0.1200  12.0110
38  C2  1   C8IM2  C22   1   0.0100  12.0110
39  HC  1   C8IM2  HC3   1   0.0600   1.0080
40  HC  1   C8IM2  HC4   1   0.0600   1.0080
41  HC  1   C8IM2  HC5   1   0.0600   1.0080
42  HC  1   C8IM2  HC6   1   0.0600   1.0080
43  HC  1   C8IM2  HC7   1   0.0600   1.0080
44  HC  1   C8IM2  HC8   1   0.0600   1.0080
45  HC  1   C8IM2  HC9   1   0.0600   1.0080
46  HC  1   C8IM2  HC10  1   0.0600   1.0080
47  HC  1   C8IM2  HC11  1   0.0600   1.0080
48  HC  1   C8IM2  HC12  1   0.0600   1.0080

[bonds]
;ai aj  f   nm  kb
 2   3  1   0.13410   435200
 2   8  1   0.13780   357400
 3   5  1   0.13780   357400
 5   6  1   0.13150   399200
 5  13  1   0.14660   282000
 6   8  1   0.13150   399200
 8   9  1   0.14660   282000
13  38  1   0.15290   224200
16  34  1   0.15290   224200
16  19  1   0.15290   224200
19  26  1   0.14660   282000
23  24  1   0.13410   435200
23  29  1   0.13780   357400
24  26  1   0.13780   357400
26  27  1   0.13150   399200
27  29  1   0.13150   399200
29  30  1   0.14660   282000
34  35  1   0.15290   224200
```

```
35  36  1   0.15290   224200
36  37  1   0.15290   224200
37  38  1   0.15290   224200
 1   2  1   0.10800   284500
 3   4  1   0.10800   284500
 6   7  1   0.10800   284500
 9  12  1   0.10900   284500
 9  10  1   0.10900   284500
 9  11  1   0.10900   284500
13  14  1   0.10900   284500
13  15  1   0.10900   284500
16  17  1   0.10900   284500
16  18  1   0.10900   284500
19  20  1   0.10900   284500
19  21  1   0.10900   284500
22  23  1   0.10800   284500
24  25  1   0.10800   284500
27  28  1   0.10800   284500
30  31  1   0.10900   284500
30  32  1   0.10900   284500
30  33  1   0.10900   284500
34  47  1   0.10900   284500
34  48  1   0.10900   284500
35  42  1   0.10900   284500
35  43  1   0.10900   284500
36  44  1   0.10900   284500
36  40  1   0.10900   284500
37  39  1   0.10900   284500
37  41  1   0.10900   284500
38  45  1   0.10900   284500
38  46  1   0.10900   284500

[angles]
;ai aj ak   f   angle   k_a
 1   2   3  1 130.90  292.9
 1   2   8  1 122.00  292.9
 3   2   8  1 107.10  585.8
 2   3   4  1 130.90  292.9
```

2	3	5	1	107.10	585.8
4	3	5	1	122.00	292.9
3	5	6	1	108.00	585.8
3	5	13	1	125.60	585.8
6	5	13	1	126.40	585.8
5	6	7	1	125.10	292.9
5	6	8	1	109.80	585.8
7	6	8	1	125.10	292.9
2	8	6	1	108.00	585.8
2	8	9	1	125.60	585.8
6	8	9	1	126.40	585.8
8	9	12	1	110.70	313.8
8	9	10	1	110.70	313.8
8	9	11	1	110.70	313.8
12	9	10	1	107.80	276.1
12	9	11	1	107.80	276.1
10	9	11	1	107.80	276.1
5	13	38	1	112.70	488.3
5	13	14	1	110.70	313.8
5	13	15	1	110.70	313.8
38	13	14	1	110.70	313.8
38	13	15	1	110.70	313.8
14	13	15	1	107.80	276.1
17	16	18	1	107.80	276.1
17	16	34	1	110.70	313.8
17	16	19	1	110.70	313.8
18	16	34	1	110.70	313.8
18	16	19	1	110.70	313.8
34	16	19	1	112.70	488.3
16	19	20	1	110.70	313.8
16	19	21	1	110.70	313.8
16	19	26	1	112.70	488.3
20	19	21	1	107.80	276.1
20	19	26	1	110.70	313.8
21	19	26	1	110.70	313.8
22	23	24	1	130.90	292.9
22	23	29	1	122.00	292.9
24	23	29	1	107.10	585.8

```
23  24  25  1 130.90  292.9
23  24  26  1 107.10  585.8
25  24  26  1 122.00  292.9
19  26  24  1 125.60  585.8
19  26  27  1 126.40  585.8
24  26  27  1 108.00  585.8
26  27  28  1 125.10  292.9
26  27  29  1 109.80  585.8
28  27  29  1 125.10  292.9
23  29  27  1 108.00  585.8
23  29  30  1 125.60  585.8
27  29  30  1 126.40  585.8
29  30  31  1 110.70  313.8
29  30  32  1 110.70  313.8
29  30  33  1 110.70  313.8
31  30  32  1 107.80  276.1
31  30  33  1 107.80  276.1
32  30  33  1 107.80  276.1
16  34  47  1 110.70  313.8
16  34  35  1 112.70  488.3
16  34  48  1 110.70  313.8
47  34  35  1 110.70  313.8
47  34  48  1 107.80  276.1
35  34  48  1 110.70  313.8
34  35  36  1 112.70  488.3
34  35  42  1 110.70  313.8
34  35  43  1 110.70  313.8
36  35  42  1 110.70  313.8
36  35  43  1 110.70  313.8
42  35  43  1 107.80  276.1
35  36  44  1 110.70  313.8
35  36  37  1 112.70  488.3
35  36  40  1 110.70  313.8
44  36  37  1 110.70  313.8
44  36  40  1 107.80  276.1
37  36  40  1 110.70  313.8
36  37  39  1 110.70  313.8
36  37  41  1 110.70  313.8
```

```
36  37  38  1 112.70  488.3
39  37  41  1 107.80  276.1
39  37  38  1 110.70  313.8
41  37  38  1 110.70  313.8
13  38  37  1 112.70  488.3
13  38  45  1 110.70  313.8
13  38  46  1 110.70  313.8
37  38  45  1 110.70  313.8
37  38  46  1 110.70  313.8
45  38  46  1 107.80  276.1

[dihedrals]
 1   2   3   4  5   0.00000 44.98000  0.00000 0.00000
 1   2   3   5  5   0.00000 44.98000  0.00000 0.00000
 8   2   3   4  5   0.00000 44.98000  0.00000 0.00000
 8   2   3   5  5   0.00000 44.98000  0.00000 0.00000
 1   2   8   6  5   0.00000 12.55000  0.00000 0.00000
 1   2   8   9  5   0.00000 12.55000  0.00000 0.00000
 3   2   8   6  5   0.00000 12.55000  0.00000 0.00000
 3   2   8   9  5   0.00000 12.55000  0.00000 0.00000
 2   3   5   6  5   0.00000 12.55000  0.00000 0.00000
 2   3   5  13  5   0.00000 12.55000  0.00000 0.00000
 4   3   5   6  5   0.00000 12.55000  0.00000 0.00000
 4   3   5  13  5   0.00000 12.55000  0.00000 0.00000
 3   5   6   7  5   0.00000 19.46000  0.00000 0.00000
 3   5   6   8  5   0.00000 19.46000  0.00000 0.00000
13   5   6   7  5   0.00000 19.46000  0.00000 0.00000
13   5   6   8  5   0.00000 19.46000  0.00000 0.00000
 3   5  13  38  5  -7.15350  6.10640  0.79390 0.00000
 3   5  13  14  5   0.00000  0.00000  0.51900 0.00000
 3   5  13  15  5   0.00000  0.00000  0.51900 0.00000
 6   5  13  38  5  -5.26910  0.00000  0.00000 0.00000
 6   5  13  14  5   0.00000  0.00000  0.00000 0.00000
 6   5  13  15  5   0.00000  0.00000  0.00000 0.00000
 5   6   8   2  5   0.00000 19.46000  0.00000 0.00000
 5   6   8   9  5   0.00000 19.46000  0.00000 0.00000
 7   6   8   2  5   0.00000 19.46000  0.00000 0.00000
 7   6   8   9  5   0.00000 19.46000  0.00000 0.00000
```

2	8	9	12	5	0.00000	0.00000	0.51900	0.00000
2	8	9	10	5	0.00000	0.00000	0.51900	0.00000
2	8	9	11	5	0.00000	0.00000	0.51900	0.00000
6	8	9	12	5	0.00000	0.00000	0.00000	0.00000
6	8	9	10	5	0.00000	0.00000	0.00000	0.00000
6	8	9	11	5	0.00000	0.00000	0.00000	0.00000
5	13	38	37	5	-7.47970	3.16420	-1.20260	0.00000
5	13	38	45	5	0.00000	0.00000	0.36700	0.00000
5	13	38	46	5	0.00000	0.00000	0.36700	0.00000
14	13	38	37	5	0.00000	0.00000	1.53130	0.00000
14	13	38	45	5	0.00000	0.00000	1.33050	0.00000
14	13	38	46	5	0.00000	0.00000	1.33050	0.00000
15	13	38	37	5	0.00000	0.00000	1.53130	0.00000
15	13	38	45	5	0.00000	0.00000	1.33050	0.00000
15	13	38	46	5	0.00000	0.00000	1.33050	0.00000
17	16	34	47	5	0.00000	0.00000	1.33050	0.00000
17	16	34	35	5	0.00000	0.00000	1.53130	0.00000
17	16	34	48	5	0.00000	0.00000	1.33050	0.00000
18	16	34	47	5	0.00000	0.00000	1.33050	0.00000
18	16	34	35	5	0.00000	0.00000	1.53130	0.00000
18	16	34	48	5	0.00000	0.00000	1.33050	0.00000
19	16	34	47	5	0.00000	0.00000	1.53130	0.00000
19	16	34	35	5	7.28000	-0.65690	1.16730	0.00000
19	16	34	48	5	0.00000	0.00000	1.53130	0.00000
17	16	19	20	5	0.00000	0.00000	1.33050	0.00000
17	16	19	21	5	0.00000	0.00000	1.33050	0.00000
17	16	19	26	5	0.00000	0.00000	0.36700	0.00000
18	16	19	20	5	0.00000	0.00000	1.33050	0.00000
18	16	19	21	5	0.00000	0.00000	1.33050	0.00000
18	16	19	26	5	0.00000	0.00000	0.36700	0.00000
34	16	19	20	5	0.00000	0.00000	1.53130	0.00000
34	16	19	21	5	0.00000	0.00000	1.53130	0.00000
34	16	19	26	5	-7.47970	3.16420	-1.20260	0.00000
16	19	26	24	5	-7.15350	6.10640	0.79390	0.00000
16	19	26	27	5	-5.26910	0.00000	0.00000	0.00000
20	19	26	24	5	0.00000	0.00000	0.51900	0.00000
20	19	26	27	5	0.00000	0.00000	0.00000	0.00000
21	19	26	24	5	0.00000	0.00000	0.51900	0.00000

21	19	26	27	5	0.00000	0.00000	0.00000	0.00000
22	23	24	25	5	0.00000	44.98000	0.00000	0.00000
22	23	24	26	5	0.00000	44.98000	0.00000	0.00000
29	23	24	25	5	0.00000	44.98000	0.00000	0.00000
29	23	24	26	5	0.00000	44.98000	0.00000	0.00000
22	23	29	27	5	0.00000	12.55000	0.00000	0.00000
22	23	29	30	5	0.00000	12.55000	0.00000	0.00000
24	23	29	27	5	0.00000	12.55000	0.00000	0.00000
24	23	29	30	5	0.00000	12.55000	0.00000	0.00000
23	24	26	19	5	0.00000	12.55000	0.00000	0.00000
23	24	26	27	5	0.00000	12.55000	0.00000	0.00000
25	24	26	19	5	0.00000	12.55000	0.00000	0.00000
25	24	26	27	5	0.00000	12.55000	0.00000	0.00000
19	26	27	28	5	0.00000	19.46000	0.00000	0.00000
19	26	27	29	5	0.00000	19.46000	0.00000	0.00000
24	26	27	28	5	0.00000	19.46000	0.00000	0.00000
24	26	27	29	5	0.00000	19.46000	0.00000	0.00000
26	27	29	23	5	0.00000	19.46000	0.00000	0.00000
26	27	29	30	5	0.00000	19.46000	0.00000	0.00000
28	27	29	23	5	0.00000	19.46000	0.00000	0.00000
28	27	29	30	5	0.00000	19.46000	0.00000	0.00000
23	29	30	31	5	0.00000	0.00000	0.51900	0.00000
23	29	30	32	5	0.00000	0.00000	0.51900	0.00000
23	29	30	33	5	0.00000	0.00000	0.51900	0.00000
27	29	30	31	5	0.00000	0.00000	0.00000	0.00000
27	29	30	32	5	0.00000	0.00000	0.00000	0.00000
27	29	30	33	5	0.00000	0.00000	0.00000	0.00000
16	34	35	36	5	7.28000	-0.65690	1.16730	0.00000
16	34	35	42	5	0.00000	0.00000	1.53130	0.00000
16	34	35	43	5	0.00000	0.00000	1.53130	0.00000
47	34	35	36	5	0.00000	0.00000	1.53130	0.00000
47	34	35	42	5	0.00000	0.00000	1.33050	0.00000
47	34	35	43	5	0.00000	0.00000	1.33050	0.00000
48	34	35	36	5	0.00000	0.00000	1.53130	0.00000
48	34	35	42	5	0.00000	0.00000	1.33050	0.00000
48	34	35	43	5	0.00000	0.00000	1.33050	0.00000
34	35	36	44	5	0.00000	0.00000	1.53130	0.00000
34	35	36	37	5	7.28000	-0.65690	1.16730	0.00000

```
34   35   36   40   5    0.00000   0.00000   1.53130 0.00000
42   35   36   44   5    0.00000   0.00000   1.33050 0.00000
42   35   36   37   5    0.00000   0.00000   1.53130 0.00000
42   35   36   40   5    0.00000   0.00000   1.33050 0.00000
43   35   36   44   5    0.00000   0.00000   1.33050 0.00000
43   35   36   37   5    0.00000   0.00000   1.53130 0.00000
43   35   36   40   5    0.00000   0.00000   1.33050 0.00000
35   36   37   39   5    0.00000   0.00000   1.53130 0.00000
35   36   37   41   5    0.00000   0.00000   1.53130 0.00000
35   36   37   38   5    7.28000  -0.65690   1.16730 0.00000
44   36   37   39   5    0.00000   0.00000   1.33050 0.00000
44   36   37   41   5    0.00000   0.00000   1.33050 0.00000
44   36   37   38   5    0.00000   0.00000   1.53130 0.00000
40   36   37   39   5    0.00000   0.00000   1.33050 0.00000
40   36   37   41   5    0.00000   0.00000   1.33050 0.00000
40   36   37   38   5    0.00000   0.00000   1.53130 0.00000
36   37   38   13   5    7.28000  -0.65690   1.16730 0.00000
36   37   38   45   5    0.00000   0.00000   1.53130 0.00000
36   37   38   46   5    0.00000   0.00000   1.53130 0.00000
39   37   38   13   5    0.00000   0.00000   1.53130 0.00000
39   37   38   45   5    0.00000   0.00000   1.33050 0.00000
39   37   38   46   5    0.00000   0.00000   1.33050 0.00000
41   37   38   13   5    0.00000   0.00000   1.53130 0.00000
41   37   38   45   5    0.00000   0.00000   1.33050 0.00000
41   37   38   46   5    0.00000   0.00000   1.33050 0.00000
```

```
;;;;;;;;;;;;;;;;;;
; bistriflimide
;;;;;;;;;;;;;;;;;;
[ moleculetype ]
TFN    3
[atoms]
;nr type    resnr   res atom    cgnr    chrg    mass
1   CBT 1   TFN    CBT1  1   0.3500   12.011
2   F1  1   TFN    F11   1  -0.1600   18.998
3   F1  1   TFN    F12   1  -0.1600   18.998
4   F1  1   TFN    F13   1  -0.1600   18.998
5   SBT 1   TFN    SBT1  1   1.0200   32.066
6   NBT 1   TFN    NBT   1  -0.6600   14.0067
7   OBT 1   TFN    OBT1  1  -0.5300   15.999
8   OBT 1   TFN    OBT2  1  -0.5300   15.999
9   SBT 1   TFN    SBT2  1   1.0200   32.066
10  OBT 1   TFN    OBT3  1  -0.5300   15.999
11  OBT 1   TFN    OBT4  1  -0.5300   15.999
12  CBT 1   TFN    CBT2  1   0.3500   12.011
13  F1  1   TFN    F14   1  -0.1600   18.998
14  F1  1   TFN    F15   1  -0.1600   18.998
15  F1  1   TFN    F16   1  -0.1600   18.998

[bonds]
;ai aj  f   nm  kb
2   1   1   0.13230   369700.0
3   1   1   0.13230   369700.0
4   1   1   0.13230   369700.0
5   1   1   0.18180   197000.0
6   5   1   0.15700   311300.0
7   5   1   0.14420   533100.0
8   5   1   0.14420   533100.0
9   6   1   0.15700   311300.0
10  9   1   0.14420   533100.0
11  9   1   0.14420   533100.0
12  9   1   0.18180   197000.0
13  12  1   0.13230   369700.0
14  12  1   0.13230   369700.0
```

```
15  12  1   0.13230   369700.0

;[ pairs ]
; i j   funct
;2   6
;3   6
;4   6

[angles]
;ai aj ak   f   angle   k_a
2   1   3   1   107.10  781.0
2   1   4   1   107.10  781.0
3   1   4   1   107.10  781.0
2   1   5   1   111.80  694.0
3   1   5   1   111.80  694.0
4   1   5   1   111.80  694.0
1   5   6   1   100.20  816.0
1   5   7   1   102.60  870.0
1   5   8   1   102.60  870.0
6   5   7   1   113.60  789.0
6   5   8   1   113.60  789.0
7   5   8   1   118.50  969.0
5   6   9   1   125.60  671.0
6   9   10  1   113.60  789.0
6   9   11  1   113.60  789.0
6   9   12  1   100.20  816.0
10  9   11  1   118.50  969.0
10  9   12  1   102.60  870.0
11  9   12  1   102.60  870.0
9   12  13  1   111.80  694.0
9   12  14  1   111.80  694.0
9   12  15  1   111.80  694.0
13  12  14  1   107.10  781.0
13  12  15  1   107.10  781.0
14  12  15  1   107.10  781.0

[dihedrals]
6   5   1   2   5   0.00000  0.00000   1.3220   0.00000
```

6	5	1	3	5	0.00000	0.00000	1.3220	0.00000
6	5	1	4	5	0.00000	0.00000	1.3220	0.00000
7	5	1	2	5	0.00000	0.00000	1.4510	0.00000
7	5	1	3	5	0.00000	0.00000	1.4510	0.00000
7	5	1	4	5	0.00000	0.00000	1.4510	0.00000
8	5	1	2	5	0.00000	0.00000	1.4510	0.00000
8	5	1	3	5	0.00000	0.00000	1.4510	0.00000
8	5	1	4	5	0.00000	0.00000	1.4510	0.00000
9	6	5	1	5	32.77300	-10.4200	-3.1950	0.00000
9	6	5	7	5	0.00000	0.00000	-0.0150	0.00000
9	6	5	8	5	0.00000	0.00000	-0.0150	0.00000
10	9	6	5	5	0.00000	0.00000	-0.0150	0.00000
11	9	6	5	5	0.00000	0.00000	-0.0150	0.00000
12	9	6	5	5	32.77300	-10.4200	-3.1950	0.00000
13	12	9	6	5	0.00000	0.00000	1.3220	0.00000
14	12	9	6	5	0.00000	0.00000	1.3220	0.00000
15	12	9	6	5	0.00000	0.00000	1.3220	0.00000
13	12	9	10	5	0.00000	0.00000	1.4510	0.00000
13	12	9	11	5	0.00000	0.00000	1.4510	0.00000
14	12	9	10	5	0.00000	0.00000	1.4510	0.00000
14	12	9	11	5	0.00000	0.00000	1.4510	0.00000
15	12	9	10	5	0.00000	0.00000	1.4510	0.00000
15	12	9	11	5	0.00000	0.00000	1.4510	0.00000

```
;;;;;;;;;;;;;;;;;;
; Zinc
;;;;;;;;;;;;;;;;;;
[ moleculetype ]
ZnX    3
[atoms]
;nr type    resnr   res atom    cgnr    chrg    mass
1   Zn  1   ZnX    Zn    1   2.0000   65.3900
```

$[C_8(mim)_2][Tf_2N]_2$ system topology

```
[ defaults ]
; nbfunc        comb-rule       gen-pairs       fudgeLJ fudgeQQ
  1             2               yes              0.5     0.5

#include "atomtypes.itp"
#include "zn.itp"
#include "c8mim2.itp"
#include "tf2n.itp"

[ system ]
; The name of the system to be simulated
Zn_Tf2N in C8mim2_Tf2N

[ molecules ]
; Molname   Number
ZnX              5
TFN            190
C8IM2           90
```

Input files for the [Choline][Tf_2N] system

```
[ atomtypes ]
; name      mass      charge      ptype      sigma      epsilon
; metallic cations
   Zn   65.39000       +2.000       A   1.95000e-01   1.04600e+00
; bistriflimide
   F1   18.99800      -0.1600       A   2.95000e-01   2.21750e-01
   CBT  12.01100       0.3500       A   3.50000e-01   2.76140e-01
   SBT  32.06600       1.0200       A   3.55000e-01   1.04600e+00
   OBT  15.99900      -0.5300       A   2.96000e-01   8.78640e-01
   NBT  14.00670      -0.6600       A   3.25000e-01   7.11280e-01
; cholinium
   C1  12.0110      -0.1700     A 3.50000e-01   2.76140e-01
   H1   1.0080       0.1300     A 2.50000e-01   1.25520e-01
   N4  14.0070       0.1200     A 3.25000e-01   7.11280e-01
   COL   12.0110       0.2750     A 3.50000e-01   2.76140e-01
   OH  15.9990      -0.6830     A 3.12000e-01   7.11280e-01
   HO   1.0080       0.4180     A 0.00000e-01   0.00000e-01
   HC   1.0080       0.0600     A 2.50000e-01   1.25520e-01
```

```
;;;;;;;;;;;;;;;;;;
; Cholinium
;;;;;;;;;;;;;;;;;;
[ moleculetype ]
CHOL    3
[atoms]
;nr type    resnr   res atom    cgnr    chrg    mass
1   N4  1   CHOL   N4    1   0.1200  14.0070
2   C1  1   CHOL   C11   1  -0.1700  12.0110
3   C1  1   CHOL   C12   1  -0.1700  12.0110
4   C1  1   CHOL   C13   1  -0.1700  12.0110
5   H1  1   CHOL   H11   1   0.1300   1.0080
6   H1  1   CHOL   H12   1   0.1300   1.0080
7   H1  1   CHOL   H13   1   0.1300   1.0080
8   H1  1   CHOL   H14   1   0.1300   1.0080
9   H1  1   CHOL   H15   1   0.1300   1.0080
10  H1  1   CHOL   H16   1   0.1300   1.0080
11  H1  1   CHOL   H17   1   0.1300   1.0080
12  H1  1   CHOL   H18   1   0.1300   1.0080
13  H1  1   CHOL   H19   1   0.1300   1.0080
14  C1  1   CHOL   C14   1  -0.1700  12.0110
15  H1  1   CHOL   H110  1   0.1300   1.0080
16  COL 1   CHOL   COL   1   0.2750  12.0110
17  H1  1   CHOL   H111  1   0.1300   1.0080
18  HC  1   CHOL   HC1   1   0.0600   1.0080
19  HC  1   CHOL   HC2   1   0.0600   1.0080
20  OH  1   CHOL   OH    1  -0.6830  15.9990
21  HO  1   CHOL   HO    1   0.4180   1.0080

[bonds]
;ai aj  f   nm  kb
 2   8  1   0.1090   284500.0
 2   9  1   0.1090   284500.0
 2  10  1   0.1090   284500.0
 3   5  1   0.1090   284500.0
 3   6  1   0.1090   284500.0
 3   7  1   0.1090   284500.0
 4  11  1   0.1090   284500.0
```

```
 4  12  1   0.1090   284500.0
 4  13  1   0.1090   284500.0
14  15  1   0.1090   284500.0
14  17  1   0.1090   284500.0
16  18  1   0.1090   284500.0
16  19  1   0.1090   284500.0
20  21  1   0.0945   284500.0
 1   2  1   0.1448   319660.0
 1   3  1   0.1448   319660.0
 1   4  1   0.1448   319660.0
 1  14  1   0.1448   319660.0
14  16  1   0.1529   224200.0
16  20  1   0.1410   267780.0

[angles]
;ai aj ak   f   angle   k_a
 2   1   3  1 107.20  433.5
 2   1   4  1 107.20  433.5
 2   1  14  1 107.20  433.5
 3   1   4  1 107.20  433.5
 3   1  14  1 107.20  433.5
 4   1  14  1 107.20  433.5
 1   2   8  1 109.50  292.9
 1   2   9  1 109.50  292.9
 1   2  10  1 109.50  292.9
 8   2   9  1 107.80  276.1
 8   2  10  1 107.80  276.1
 9   2  10  1 107.80  276.1
 1   3   5  1 109.50  292.9
 1   3   6  1 109.50  292.9
 1   3   7  1 109.50  292.9
 5   3   6  1 107.80  276.1
 5   3   7  1 107.80  276.1
 6   3   7  1 107.80  276.1
 1   4  11  1 109.50  292.9
 1   4  12  1 109.50  292.9
 1   4  13  1 109.50  292.9
11   4  12  1 107.80  276.1
```

```
11   4  13  1 107.80  276.1
12   4  13  1 107.80  276.1
 1  14  15  1 109.50  292.9
 1  14  16  1 109.50  470.3
 1  14  17  1 109.50  292.9
15  14  16  1 110.70  313.8
15  14  17  1 107.80  276.1
16  14  17  1 110.70  313.8
14  16  18  1 110.70  313.8
14  16  19  1 110.70  313.8
14  16  20  1 109.50  418.4
18  16  19  1 107.80  276.1
18  16  20  1 109.50  292.9
19  16  20  1 109.50  292.9
16  20  21  1 108.50  460.2

[dihedrals]
 3   1   2   8  5     0.0000   0.0000   2.3430   0.00000
 3   1   2   9  5     0.0000   0.0000   2.3430   0.00000
 3   1   2  10  5     0.0000   0.0000   2.3430   0.00000
 4   1   2   8  5     0.0000   0.0000   2.3430   0.00000
 4   1   2   9  5     0.0000   0.0000   2.3430   0.00000
 4   1   2  10  5     0.0000   0.0000   2.3430   0.00000
14   1   2   8  5     0.0000   0.0000   2.3430   0.00000
14   1   2   9  5     0.0000   0.0000   2.3430   0.00000
14   1   2  10  5     0.0000   0.0000   2.3430   0.00000
 2   1   3   5  5     0.0000   0.0000   2.3430   0.00000
 2   1   3   6  5     0.0000   0.0000   2.3430   0.00000
 2   1   3   7  5     0.0000   0.0000   2.3430   0.00000
 4   1   3   5  5     0.0000   0.0000   2.3430   0.00000
 4   1   3   6  5     0.0000   0.0000   2.3430   0.00000
 4   1   3   7  5     0.0000   0.0000   2.3430   0.00000
14   1   3   5  5     0.0000   0.0000   2.3430   0.00000
14   1   3   6  5     0.0000   0.0000   2.3430   0.00000
14   1   3   7  5     0.0000   0.0000   2.3430   0.00000
 2   1   4  11  5     0.0000   0.0000   2.3430   0.00000
 2   1   4  12  5     0.0000   0.0000   2.3430   0.00000
 2   1   4  13  5     0.0000   0.0000   2.3430   0.00000
```

3	1	4	11	5	0.0000	0.0000	2.3430	0.00000
3	1	4	12	5	0.0000	0.0000	2.3430	0.00000
3	1	4	13	5	0.0000	0.0000	2.3430	0.00000
14	1	4	11	5	0.0000	0.0000	2.3430	0.00000
14	1	4	12	5	0.0000	0.0000	2.3430	0.00000
14	1	4	13	5	0.0000	0.0000	2.3430	0.00000
2	1	14	15	5	0.0000	0.0000	2.3430	0.00000
2	1	14	16	5	1.7405	-0.5356	2.9079	0.00000
2	1	14	17	5	0.0000	0.0000	2.3430	0.00000
3	1	14	15	5	0.0000	0.0000	2.3430	0.00000
3	1	14	16	5	1.7405	-0.5356	2.9079	0.00000
3	1	14	17	5	0.0000	0.0000	2.3430	0.00000
4	1	14	15	5	0.0000	0.0000	2.3430	0.00000
4	1	14	16	5	1.7405	-0.5356	2.9079	0.00000
4	1	14	17	5	0.0000	0.0000	2.3430	0.00000
1	14	16	18	5	-4.2384	-2.9665	1.9790	0.00000
1	14	16	19	5	-4.2384	-2.9665	1.9790	0.00000
1	14	16	20	5	-44.0515	-5.4349	0.0000	0.00000
15	14	16	18	5	0.0000	0.0000	1.2552	0.00000
15	14	16	19	5	0.0000	0.0000	1.2552	0.00000
15	14	16	20	5	0.0000	0.0000	1.9581	0.00000
17	14	16	18	5	0.0000	0.0000	1.2552	0.00000
17	14	16	19	5	0.0000	0.0000	1.2552	0.00000
17	14	16	20	5	0.0000	0.0000	1.9581	0.00000
14	16	20	21	5	-1.4895	-0.7280	2.0585	0.00000
18	16	20	21	5	0.0000	0.0000	1.8828	0.00000
19	16	20	21	5	0.0000	0.0000	1.8828	0.00000

```
;;;;;;;;;;;;;;;;;;
; bistriflimide
;;;;;;;;;;;;;;;;;;
[ moleculetype ]
TFN    3
[atoms]
;nr type    resnr   res atom    cgnr    chrg    mass
1   CBT 1   TFN    CBT1  1   0.3500   12.011
2   F1  1   TFN    F11   1  -0.1600   18.998
3   F1  1   TFN    F12   1  -0.1600   18.998
4   F1  1   TFN    F13   1  -0.1600   18.998
5   SBT 1   TFN    SBT1  1   1.0200   32.066
6   NBT 1   TFN    NBT   1  -0.6600   14.0067
7   OBT 1   TFN    OBT1  1  -0.5300   15.999
8   OBT 1   TFN    OBT2  1  -0.5300   15.999
9   SBT 1   TFN    SBT2  1   1.0200   32.066
10  OBT 1   TFN    OBT3  1  -0.5300   15.999
11  OBT 1   TFN    OBT4  1  -0.5300   15.999
12  CBT 1   TFN    CBT2  1   0.3500   12.011
13  F1  1   TFN    F14   1  -0.1600   18.998
14  F1  1   TFN    F15   1  -0.1600   18.998
15  F1  1   TFN    F16   1  -0.1600   18.998

[bonds]
;ai aj  f   nm  kb
2   1   1   0.13230   369700.0
3   1   1   0.13230   369700.0
4   1   1   0.13230   369700.0
5   1   1   0.18180   197000.0
6   5   1   0.15700   311300.0
7   5   1   0.14420   533100.0
8   5   1   0.14420   533100.0
9   6   1   0.15700   311300.0
10  9   1   0.14420   533100.0
11  9   1   0.14420   533100.0
12  9   1   0.18180   197000.0
13  12  1   0.13230   369700.0
14  12  1   0.13230   369700.0
```

```
15  12  1   0.13230   369700.0

;[ pairs ]
; i j   funct
;2   6
;3   6
;4   6

[angles]
;ai aj ak   f   angle   k_a
2   1   3   1   107.10  781.0
2   1   4   1   107.10  781.0
3   1   4   1   107.10  781.0
2   1   5   1   111.80  694.0
3   1   5   1   111.80  694.0
4   1   5   1   111.80  694.0
1   5   6   1   100.20  816.0
1   5   7   1   102.60  870.0
1   5   8   1   102.60  870.0
6   5   7   1   113.60  789.0
6   5   8   1   113.60  789.0
7   5   8   1   118.50  969.0
5   6   9   1   125.60  671.0
6   9   10  1   113.60  789.0
6   9   11  1   113.60  789.0
6   9   12  1   100.20  816.0
10  9   11  1   118.50  969.0
10  9   12  1   102.60  870.0
11  9   12  1   102.60  870.0
9   12  13  1   111.80  694.0
9   12  14  1   111.80  694.0
9   12  15  1   111.80  694.0
13  12  14  1   107.10  781.0
13  12  15  1   107.10  781.0
14  12  15  1   107.10  781.0

[dihedrals]
6   5   1   2   5   0.00000  0.00000   1.3220   0.00000
```

6	5	1	3	5	0.00000	0.00000	1.3220	0.00000
6	5	1	4	5	0.00000	0.00000	1.3220	0.00000
7	5	1	2	5	0.00000	0.00000	1.4510	0.00000
7	5	1	3	5	0.00000	0.00000	1.4510	0.00000
7	5	1	4	5	0.00000	0.00000	1.4510	0.00000
8	5	1	2	5	0.00000	0.00000	1.4510	0.00000
8	5	1	3	5	0.00000	0.00000	1.4510	0.00000
8	5	1	4	5	0.00000	0.00000	1.4510	0.00000
9	6	5	1	5	32.77300	-10.4200	-3.1950	0.00000
9	6	5	7	5	0.00000	0.00000	-0.0150	0.00000
9	6	5	8	5	0.00000	0.00000	-0.0150	0.00000
10	9	6	5	5	0.00000	0.00000	-0.0150	0.00000
11	9	6	5	5	0.00000	0.00000	-0.0150	0.00000
12	9	6	5	5	32.77300	-10.4200	-3.1950	0.00000
13	12	9	6	5	0.00000	0.00000	1.3220	0.00000
14	12	9	6	5	0.00000	0.00000	1.3220	0.00000
15	12	9	6	5	0.00000	0.00000	1.3220	0.00000
13	12	9	10	5	0.00000	0.00000	1.4510	0.00000
13	12	9	11	5	0.00000	0.00000	1.4510	0.00000
14	12	9	10	5	0.00000	0.00000	1.4510	0.00000
14	12	9	11	5	0.00000	0.00000	1.4510	0.00000
15	12	9	10	5	0.00000	0.00000	1.4510	0.00000
15	12	9	11	5	0.00000	0.00000	1.4510	0.00000

```
;;;;;;;;;;;;;;;;;;
; Zinc
;;;;;;;;;;;;;;;;;;
[ moleculetype ]
ZnX    3
[atoms]
;nr type    resnr   res atom    cgnr    chrg    mass
1   Zn  1   ZnX    Zn    1   2.0000   65.3900
```

[Choline][Tf_2N] system topology

```
[ defaults ]
; nbfunc        comb-rule       gen-pairs       fudgeLJ fudgeQQ
  1             2               yes              0.5     0.5

#include "atomtypes.itp"
#include "zn.itp"
#include "cholinium.itp"
#include "tf2n.itp"

[ system ]
; The name of the system to be simulated
Zn_Tf2N in cholinium_Tf2N

[ molecules ]
; Molname   Number
ZnX              5
TFN            205
CHOL           195
```

Input files for the [BTMA][Tf_2N] system

```
[ atomtypes ]
; name      mass      charge      ptype      sigma      epsilon
; metallic cations
   Zn   65.39000       +2.000       A   1.95000e-01   1.04600e+00
; bistriflimide
   F1   18.99800      -0.1600       A   2.95000e-01   2.21750e-01
   CBT  12.01100       0.3500       A   3.50000e-01   2.76140e-01
   SBT  32.06600       1.0200       A   3.55000e-01   1.04600e+00
   OBT  15.99900      -0.5300       A   2.96000e-01   8.78640e-01
   NBT  14.00670      -0.6600       A   3.25000e-01   7.11280e-01
; butyltrimethylammonium
   N4  14.0070       0.1200     A 3.25000e-01   7.11280e-01
   C1  12.0110      -0.1700     A 3.50000e-01   2.76140e-01
   H1   1.0080       0.1300     A 2.50000e-01   1.25520e-01
   C2 12.01100       0.0100     A 3.50000e-01   2.76140e-01
   CS 12.01100      -0.1200     A 3.50000e-01   2.76140e-01
   CT 12.01100      -0.1800     A 3.50000e-01   2.76140e-01
   HC    1.00800       0.0600       A   2.50000e-01   1.25520e-01
```

```
;;;;;;;;;;;;;;;;;;
; Butyltrimethylammonium
;;;;;;;;;;;;;;;;;;
[ moleculetype ]
BTMA    3
[atoms]
;nr type    resnr   res atom    cgnr    chrg    mass
1   N4  1   BTMA   N4    1   0.1200  14.0070
2   C1  1   BTMA   C11   1  -0.1700  12.0110
3   C1  1   BTMA   C12   1  -0.1700  12.0110
4   C1  1   BTMA   C13   1  -0.1700  12.0110
5   C1  1   BTMA   C14   1  -0.1700  12.0110
6   C2  1   BTMA   C2    1   0.0100  12.0110
7   CS  1   BTMA   CS    1  -0.1200  12.0110
8   CT  1   BTMA   CT    1  -0.1800  12.0110
9   H1  1   BTMA   H11   1   0.1300   1.0080
10  H1  1   BTMA   H12   1   0.1300   1.0080
11  H1  1   BTMA   H13   1   0.1300   1.0080
12  H1  1   BTMA   H14   1   0.1300   1.0080
13  H1  1   BTMA   H15   1   0.1300   1.0080
14  H1  1   BTMA   H16   1   0.1300   1.0080
15  H1  1   BTMA   H17   1   0.1300   1.0080
16  H1  1   BTMA   H18   1   0.1300   1.0080
17  H1  1   BTMA   H19   1   0.1300   1.0080
18  H1  1   BTMA   H110  1   0.1300   1.0080
19  H1  1   BTMA   H111  1   0.1300   1.0080
20  HC  1   BTMA   HC1   1   0.0600   1.0080
21  HC  1   BTMA   HC2   1   0.0600   1.0080
22  HC  1   BTMA   HC3   1   0.0600   1.0080
23  HC  1   BTMA   HC4   1   0.0600   1.0080
24  HC  1   BTMA   HC5   1   0.0600   1.0080
25  HC  1   BTMA   HC6   1   0.0600   1.0080
26  HC  1   BTMA   HC7   1   0.0600   1.0080

[bonds]
;ai aj  f   nm  kb
 2   9  1   0.1090  284500.0
 2  10  1   0.1090  284500.0
```

```
 2  11  1   0.1090  284500.0
 3  12  1   0.1090  284500.0
 3  13  1   0.1090  284500.0
 3  14  1   0.1090  284500.0
 4  15  1   0.1090  284500.0
 4  16  1   0.1090  284500.0
 4  17  1   0.1090  284500.0
 5  18  1   0.1090  284500.0
 5  19  1   0.1090  284500.0
 6  20  1   0.1090  284500.0
 6  21  1   0.1090  284500.0
 7  22  1   0.1090  284500.0
 7  23  1   0.1090  284500.0
 8  24  1   0.1090  284500.0
 8  25  1   0.1090  284500.0
 8  26  1   0.1090  284500.0
 1   2  1   0.1448  319660.0
 1   3  1   0.1448  319660.0
 1   4  1   0.1448  319660.0
 1   5  1   0.1448  319660.0
 5   6  1   0.1529  224200.0
 6   7  1   0.1529  224200.0
 7   8  1   0.1529  224200.0

[angles]
;ai aj ak   f   angle   k_a
 2   1   3  1 107.20  433.5
 2   1   4  1 107.20  433.5
 2   1   5  1 107.20  433.5
 3   1   4  1 107.20  433.5
 3   1   5  1 107.20  433.5
 4   1   5  1 107.20  433.5
 1   2   9  1 109.50  292.9
 1   2  10  1 109.50  292.9
 1   2  11  1 109.50  292.9
 9   2  10  1 107.80  276.1
 9   2  11  1 107.80  276.1
10   2  11  1 107.80  276.1
```

```
 1   3  12  1 109.50  292.9
 1   3  13  1 109.50  292.9
 1   3  14  1 109.50  292.9
12   3  13  1 107.80  276.1
12   3  14  1 107.80  276.1
13   3  14  1 107.80  276.1
 1   4  15  1 109.50  292.9
 1   4  16  1 109.50  292.9
 1   4  17  1 109.50  292.9
15   4  16  1 107.80  276.1
15   4  17  1 107.80  276.1
16   4  17  1 107.80  276.1
 1   5   6  1 109.50  470.3
 1   5  18  1 109.50  292.9
 1   5  19  1 109.50  292.9
 6   5  18  1 110.70  313.8
 6   5  19  1 110.70  313.8
18   5  19  1 107.80  276.1
 5   6   7  1 112.70  488.3
 5   6  20  1 110.70  313.8
 5   6  21  1 110.70  313.8
 7   6  20  1 110.70  313.8
 7   6  21  1 110.70  313.8
20   6  21  1 107.80  276.1
 6   7   8  1 112.70  488.3
 6   7  22  1 110.70  313.8
 6   7  23  1 110.70  313.8
 8   7  22  1 110.70  313.8
 8   7  23  1 110.70  313.8
22   7  23  1 107.80  276.1
 7   8  24  1 110.70  313.8
 7   8  25  1 110.70  313.8
 7   8  26  1 110.70  313.8
24   8  25  1 107.80  276.1
24   8  26  1 107.80  276.1
25   8  26  1 107.80  276.1

[dihedrals]
```

```
3   1   2   9  5     0.0000 0.0000    2.3430    0.00000
3   1   2  10  5     0.0000 0.0000    2.3430    0.00000
3   1   2  11  5     0.0000 0.0000    2.3430    0.00000
4   1   2   9  5     0.0000 0.0000    2.3430    0.00000
4   1   2  10  5     0.0000 0.0000    2.3430    0.00000
4   1   2  11  5     0.0000 0.0000    2.3430    0.00000
5   1   2   9  5     0.0000 0.0000    2.3430    0.00000
5   1   2  10  5     0.0000 0.0000    2.3430    0.00000
5   1   2  11  5     0.0000 0.0000    2.3430    0.00000
2   1   3  12  5     0.0000 0.0000    2.3430    0.00000
2   1   3  13  5     0.0000 0.0000    2.3430    0.00000
2   1   3  14  5     0.0000 0.0000    2.3430    0.00000
4   1   3  12  5     0.0000 0.0000    2.3430    0.00000
4   1   3  13  5     0.0000 0.0000    2.3430    0.00000
4   1   3  14  5     0.0000 0.0000    2.3430    0.00000
5   1   3  12  5     0.0000 0.0000    2.3430    0.00000
5   1   3  13  5     0.0000 0.0000    2.3430    0.00000
5   1   3  14  5     0.0000 0.0000    2.3430    0.00000
2   1   4  15  5     0.0000 0.0000    2.3430    0.00000
2   1   4  16  5     0.0000 0.0000    2.3430    0.00000
2   1   4  17  5     0.0000 0.0000    2.3430    0.00000
3   1   4  15  5     0.0000 0.0000    2.3430    0.00000
3   1   4  16  5     0.0000 0.0000    2.3430    0.00000
3   1   4  17  5     0.0000 0.0000    2.3430    0.00000
5   1   4  15  5     0.0000 0.0000    2.3430    0.00000
5   1   4  16  5     0.0000 0.0000    2.3430    0.00000
5   1   4  17  5     0.0000 0.0000    2.3430    0.00000
2   1   5   6  5     1.7405   -0.5356    2.9079    0.00000
2   1   5  18  5     0.0000 0.0000    2.3430    0.00000
2   1   5  19  5     0.0000 0.0000    2.3430    0.00000
3   1   5   6  5     1.7405   -0.5356    2.9079    0.00000
3   1   5  18  5     0.0000 0.0000    2.3430    0.00000
3   1   5  19  5     0.0000 0.0000    2.3430    0.00000
4   1   5   6  5     1.7405   -0.5356    2.9079    0.00000
4   1   5  18  5     0.0000 0.0000    2.3430    0.00000
4   1   5  19  5     0.0000 0.0000    2.3430    0.00000
1   5   6   7  5    10.0081   -2.8200    2.3012    0.00000
1   5   6  20  5    -4.2384   -2.9665    1.9790    0.00000
```

```
 1   5   6  21   5    -4.2384   -2.9665    1.9790    0.00000
18   5   6   7   5     0.0000 0.0000    1.2552    0.00000
18   5   6  20   5     0.0000 0.0000    1.2552    0.00000
18   5   6  21   5     0.0000 0.0000    1.2552    0.00000
19   5   6   7   5     0.0000 0.0000    1.2552    0.00000
19   5   6  20   5     0.0000 0.0000    1.2552    0.00000
19   5   6  21   5     0.0000 0.0000    1.2552    0.00000
 5   6   7   8   5     5.4392   -0.2092    0.8368    0.00000
 5   6   7  22   5     0.0000 0.0000    1.2552    0.00000
 5   6   7  23   5     0.0000 0.0000    1.2552    0.00000
20   6   7   8   5     0.0000 0.0000    1.2552    0.00000
20   6   7  22   5     0.0000 0.0000    1.2552    0.00000
20   6   7  23   5     0.0000 0.0000    1.2552    0.00000
21   6   7   8   5     0.0000 0.0000    1.2552    0.00000
21   6   7  22   5     0.0000 0.0000    1.2552    0.00000
21   6   7  23   5     0.0000 0.0000    1.2552    0.00000
 6   7   8  24   5     0.0000 0.0000    1.2552    0.00000
 6   7   8  25   5     0.0000 0.0000    1.2552    0.00000
 6   7   8  26   5     0.0000 0.0000    1.2552    0.00000
22   7   8  24   5     0.0000 0.0000    1.2552    0.00000
22   7   8  25   5     0.0000 0.0000    1.2552    0.00000
22   7   8  26   5     0.0000 0.0000    1.2552    0.00000
23   7   8  24   5     0.0000 0.0000    1.2552    0.00000
23   7   8  25   5     0.0000 0.0000    1.2552    0.00000
23   7   8  26   5     0.0000 0.0000    1.2552    0.00000
```

```
;;;;;;;;;;;;;;;;;;
; bistriflimide
;;;;;;;;;;;;;;;;;;
[ moleculetype ]
TFN    3
[atoms]
;nr type    resnr   res atom    cgnr    chrg    mass
1   CBT 1   TFN    CBT1  1   0.3500   12.011
2   F1  1   TFN    F11   1  -0.1600   18.998
3   F1  1   TFN    F12   1  -0.1600   18.998
4   F1  1   TFN    F13   1  -0.1600   18.998
5   SBT 1   TFN    SBT1  1   1.0200   32.066
6   NBT 1   TFN    NBT   1  -0.6600   14.0067
7   OBT 1   TFN    OBT1  1  -0.5300   15.999
8   OBT 1   TFN    OBT2  1  -0.5300   15.999
9   SBT 1   TFN    SBT2  1   1.0200   32.066
10  OBT 1   TFN    OBT3  1  -0.5300   15.999
11  OBT 1   TFN    OBT4  1  -0.5300   15.999
12  CBT 1   TFN    CBT2  1   0.3500   12.011
13  F1  1   TFN    F14   1  -0.1600   18.998
14  F1  1   TFN    F15   1  -0.1600   18.998
15  F1  1   TFN    F16   1  -0.1600   18.998

[bonds]
;ai aj  f   nm  kb
2   1   1   0.13230   369700.0
3   1   1   0.13230   369700.0
4   1   1   0.13230   369700.0
5   1   1   0.18180   197000.0
6   5   1   0.15700   311300.0
7   5   1   0.14420   533100.0
8   5   1   0.14420   533100.0
9   6   1   0.15700   311300.0
10  9   1   0.14420   533100.0
11  9   1   0.14420   533100.0
12  9   1   0.18180   197000.0
13  12  1   0.13230   369700.0
14  12  1   0.13230   369700.0
```

```
15  12  1   0.13230   369700.0

;[ pairs ]
; i j   funct
;2   6
;3   6
;4   6

[angles]
;ai aj ak   f   angle   k_a
2   1   3   1   107.10  781.0
2   1   4   1   107.10  781.0
3   1   4   1   107.10  781.0
2   1   5   1   111.80  694.0
3   1   5   1   111.80  694.0
4   1   5   1   111.80  694.0
1   5   6   1   100.20  816.0
1   5   7   1   102.60  870.0
1   5   8   1   102.60  870.0
6   5   7   1   113.60  789.0
6   5   8   1   113.60  789.0
7   5   8   1   118.50  969.0
5   6   9   1   125.60  671.0
6   9   10  1   113.60  789.0
6   9   11  1   113.60  789.0
6   9   12  1   100.20  816.0
10  9   11  1   118.50  969.0
10  9   12  1   102.60  870.0
11  9   12  1   102.60  870.0
9   12  13  1   111.80  694.0
9   12  14  1   111.80  694.0
9   12  15  1   111.80  694.0
13  12  14  1   107.10  781.0
13  12  15  1   107.10  781.0
14  12  15  1   107.10  781.0

[dihedrals]
6   5   1   2   5   0.00000  0.00000   1.3220   0.00000
```

6	5	1	3	5	0.00000	0.00000	1.3220	0.00000
6	5	1	4	5	0.00000	0.00000	1.3220	0.00000
7	5	1	2	5	0.00000	0.00000	1.4510	0.00000
7	5	1	3	5	0.00000	0.00000	1.4510	0.00000
7	5	1	4	5	0.00000	0.00000	1.4510	0.00000
8	5	1	2	5	0.00000	0.00000	1.4510	0.00000
8	5	1	3	5	0.00000	0.00000	1.4510	0.00000
8	5	1	4	5	0.00000	0.00000	1.4510	0.00000
9	6	5	1	5	32.77300	-10.4200	-3.1950	0.00000
9	6	5	7	5	0.00000	0.00000	-0.0150	0.00000
9	6	5	8	5	0.00000	0.00000	-0.0150	0.00000
10	9	6	5	5	0.00000	0.00000	-0.0150	0.00000
11	9	6	5	5	0.00000	0.00000	-0.0150	0.00000
12	9	6	5	5	32.77300	-10.4200	-3.1950	0.00000
13	12	9	6	5	0.00000	0.00000	1.3220	0.00000
14	12	9	6	5	0.00000	0.00000	1.3220	0.00000
15	12	9	6	5	0.00000	0.00000	1.3220	0.00000
13	12	9	10	5	0.00000	0.00000	1.4510	0.00000
13	12	9	11	5	0.00000	0.00000	1.4510	0.00000
14	12	9	10	5	0.00000	0.00000	1.4510	0.00000
14	12	9	11	5	0.00000	0.00000	1.4510	0.00000
15	12	9	10	5	0.00000	0.00000	1.4510	0.00000
15	12	9	11	5	0.00000	0.00000	1.4510	0.00000

```
;;;;;;;;;;;;;;;;;;
; Zinc
;;;;;;;;;;;;;;;;;;
[ moleculetype ]
ZnX    3
[atoms]
;nr type    resnr   res atom    cgnr    chrg    mass
1   Zn  1   ZnX    Zn    1   2.0000   65.3900
```

[BTMA][Tf_2N] system topology

```
[ defaults ]
; nbfunc        comb-rule       gen-pairs       fudgeLJ fudgeQQ
  1             2               yes              0.5     0.5

#include "atomtypes.itp"
#include "zn.itp"
#include "bume3n.itp"
#include "tf2n.itp"

[ system ]
; The name of the system to be simulated
Zn_Tf2N in BuMe3N_Tf2N

[ molecules ]
; Molname   Number
ZnX              5
TFN            185
BTMA           175
```