Electronic Supplementary Material (ESI) for Soft Matter.

Force Field Files

Cations

c4mim.itp

```
[ moleculetype ]
; Name              nrexcl
 BMI               3

[ atoms ]
;   nr       type  resnr residue  atom   cgnr     charge       mass
     1         CR      1    BMI     Z1      1      0.0000    13.0190
     2         H5      1    BMI     Z2      2      0.1500     1.0079
     3         CW      1    BMI     Z3      3     -0.1600    13.0190
     4         H4      1    BMI     Z4      4      0.2000     1.0079
     5         CW      1    BMI     Z5      5     -0.1600    13.0190
     6         H4      1    BMI     Z6      6      0.2000     1.0079
     7         NA      1    BMI     Z7      7      0.0150    14.0067
     8         NA      1    BMI     Z8      8      0.0150    14.0067
     9        CN3      1    BMI     Z9      9      0.2600    15.0350
    10        CN2      1    BMI    Z10     10      0.2300    14.0270
    11        CTA      1    BMI    Z11     11      0.0500    14.0270
    12        CT2      1    BMI    Z12     12      0.0000    14.0270
    13        CT3      1    BMI    Z13     13      0.0000    15.0350

[ bonds ]
;  ai    aj   funct          r         k
     1     2     1     0.10700    2.8811e+05
     1     7     1     0.13250    3.4401e+05
     1     8     1     0.13250    3.4401e+05
     3     4     1     0.10700    2.8811e+05
     3     5     1     0.13430    4.0033e+05
     3     7     1     0.13780    3.4401e+05
     5     6     1     0.10700    2.8811e+05
     5     8     1     0.13780    3.4401e+05
     7     9     1     0.15000    2.1631e+05
     8    10     1     0.14920    2.1631e+05
    10    11     1     0.16100    1.6284e+05
    11    12     1     0.16100    1.6284e+05
    12    13     1     0.16100    2.1631e+05

[ pairs ]
;  ai    aj     funct
     1      4      1
     1      6      1
     1     11      1
     2      3      1
     2      9      1
     2      5      1
     2     10      1
     3     10      1
     4      6      1
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     4      8      1
     4      9      1
     5      9      1
     5     11      1
     6      7      1
     6     10      1
     7     10      1
     8      9      1
     8     12      1
    10     13      1

[ angles ]
;  ai    aj    ak    funct     theta       cth
     2     1     7     1  1.2570e+02  4.2844e+02
     2     1     8     1  1.2570e+02  4.2844e+02
     7     1     8     1  1.0990e+02  6.1672e+02
     4     3     5     1  1.3070e+02  4.1840e+02
     4     3     7     1  1.2210e+02  4.2844e+02
     5     3     7     1  1.0710e+02  5.8409e+02
     3     5     6     1  1.3070e+02  4.1840e+02
     3     5     8     1  1.0710e+02  5.8409e+02
     6     5     8     1  1.2210e+02  4.2844e+02
     1     7     3     1  1.0800e+02  5.6735e+02
     1     7     9     1  1.2630e+02  5.3723e+02
     3     7     9     1  1.2570e+02  5.3723e+02
     1     8     5     1  1.0800e+02  5.6735e+02
     1     8    10     1  1.2630e+02  5.3723e+02
     5     8    10     1  1.2570e+02  5.3723e+02
     8    10    11     1  1.1220e+02  6.6944e+02
    10    11    12     1  1.0220e+02  7.8324e+02
    11    12    13     1  1.0480e+02  9.5060e+02

[ dihedrals ]
;    ai    aj    ak    al funct  theta        cth     mult
     1     7     3     4     1   180.0      8.3680      2;
     1     7     3     5     1   180.0     50.2080      2;
     1     8     5     3     1   180.0     50.2080      2;
     1     8     5     6     1   180.0      8.3680      2;
     1     8    10    11     9     0.0      0.0711      1;
     1     8    10    11     9   180.0      0.0628      2;
     1     8    10    11     9     0.0     -0.8870      3;
     2     1     7     3     1   180.0      6.2760      2;
     2     1     7     9     1   180.0      6.2760      2;
     2     1     8     5     1   180.0      6.2760      2;
     2     1     8    10     1   180.0      6.2760      2;
     3     5     8    10     1   180.0      8.3680      2;
     3     7     1     8     1   180.0     50.2080      2;
     4     3     5     6     1   180.0      6.2760      2;
     4     3     5     8     1   180.0      6.2760      2;
     4     3     7     9     1   180.0      6.2760      2;
     5     3     7     9     1   180.0      8.3680      2;
     5     8     1     7     1   180.0     50.2080      2;
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     5     8    10    11     9     0.0      0.8075      1;
     5     8    10    11     9   180.0      0.9205      2;
     5     8    10    11     9     0.0      0.0377      3;
     6     5     3     7     1   180.0      6.2760      2;
     6     5     8    10     1   180.0      6.2760      2;
     7     1     8    10     1   180.0      8.3680      2;
     7     3     5     8     1   180.0     50.2080      2;
     8     1     7     9     1   180.0      8.3680      2;
    10    11    12    13     9     0.0    -14.6440      1;
    10    11    12    13     9   180.0      6.6944      2;
    10    11    12    13     9     0.0      6.6944      3;
     1     3     7     9     4   180.0      8.3680      2;
     1     5     8    10     4   180.0      8.3680      2;
     7     5     3     4     4   180.0      4.6024      2;
     7     8     1     2     4   180.0      4.6024      2;
     8     3     5     6     4   180.0      4.6024      2;
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c8mim.itp

```
[ moleculetype ]
; Name              nrexcl
OMI                 3

[ atoms ]
;   nr       type  resnr residue  atom   cgnr     charge       mass
     1         CR      1   OMI     C1      1      0.0000    13.0190
     2         H5      1   OMI     H2      2      0.1500     1.0079
     3         CW      1   OMI     C3      3     -0.1600    13.0190
     4         H4      1   OMI     H4      4      0.2000     1.0079
     5         CW      1   OMI     C5      5     -0.1600    13.0190
     6         H4      1   OMI     H6      6      0.2000     1.0079
     7         NA      1   OMI     N7      7      0.0150    14.0067
     8         NA      1   OMI     N8      8      0.0150    14.0067
     9        CN3      1   OMI     C9      9      0.2600    15.0350
    10        CN2      1   OMI    C10     10      0.2300    14.0270
    11        CTA      1   OMI    C11     11      0.0500    14.0270
    12        CT2      1   OMI    C12     12      0.0000    14.0270
    13        CT2      1   OMI    C13     13      0.0000    14.0270
    14        CT2      1   OMI    C14     14      0.0000    14.0270
    15        CT2      1   OMI    C15     15      0.0000    14.0270
    16        CT2      1   OMI    C16     16      0.0000    14.0270
    17        CT3      1   OMI    C17     17      0.0000    15.0350

[ bonds ]
;  ai    aj   funct          r         k
     1     2     1     0.10700    2.8811e+05
     1     7     1     0.13250    3.4401e+05
     1     8     1     0.13250    3.4401e+05
     3     4     1     0.10700    2.8811e+05
     3     5     1     0.13430    4.0033e+05
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     3     8     1     0.13780    3.4401e+05
     5     6     1     0.10700    2.8811e+05
     5     7     1     0.13780    3.4401e+05
     7    10     1     0.14920    2.1631e+05
     8     9     1     0.15000    2.1631e+05
    10    11     1     0.16100    1.6284e+05
    11    12     1     0.16100    1.6284e+05
    12    13     1     0.16100    1.6284e+05
    13    14     1     0.16100    1.6284e+05
    14    15     1     0.16100    1.6284e+05
    15    16     1     0.16100    1.6284e+05
    16    17     1     0.16100    2.1840e+05

[ pairs ]
;  ai    aj     funct
     1      6      1
     1     11      1
     1      4      1
     2      5      1
     2     10      1
     2      3      1
     2      9      1
     3     10      1
     4      6      1
     4      7      1
     4      9      1
     5      9      1
     5     11      1
     6      8      1
     6     10      1
     7      9      1
     7     12      1
     8     10      1
    10     13      1
    11     14      1
    12     15      1
    13     16      1
    14     17      1

[ angles ]
;  ai    aj    ak    funct     theta       cth
     2     1     7     1  1.2570e+02  4.2844e+02
     2     1     8     1  1.2570e+02  4.2844e+02
     7     1     8     1  1.0990e+02  6.1672e+02
     4     3     5     1  1.3070e+02  4.1840e+02
     4     3     8     1  1.2210e+02  4.2844e+02
     5     3     8     1  1.0710e+02  5.8409e+02
     3     5     6     1  1.3070e+02  4.1840e+02
     3     5     7     1  1.0710e+02  5.8409e+02
     6     5     7     1  1.2210e+02  4.2844e+02
     1     7     5     1  1.0800e+02  5.6735e+02
     1     7    10     1  1.2630e+02  5.3723e+02
```

```
     5     7    10     1  1.2570e+02  5.3723e+02
     1     8     3     1  1.0800e+02  5.6735e+02
     1     8     9     1  1.2630e+02  5.3723e+02
     3     8     9     1  1.2570e+02  5.3723e+02
     7    10    11     1  1.1220e+02  6.6944e+02
    10    11    12     1  1.0220e+02  7.8324e+02
    11    12    13     1  1.0220e+02  7.8324e+02
    12    13    14     1  1.0220e+02  7.8324e+02
    13    14    15     1  1.0220e+02  7.8324e+02
    14    15    16     1  1.0220e+02  7.8324e+02
    15    16    17     1  1.0480e+02  9.5060e+02

[ dihedrals ]
;    ai    aj    ak    al funct  theta        cth     mult
     1     7     5     3     1   180.0     50.2080      2;
     1     7     5     6     1   180.0      8.3680      2;
     1     7    10    11     9     0.0      0.0711      1;
     1     7    10    11     9   180.0      0.06276     2;
     1     7    10    11     9     0.0      0.8870      3;
     1     8     3     4     1   180.0      8.3680      2;
     1     8     3     5     1   180.0     50.2080      2;
     2     1     7     5     1   180.0      6.2760      2;
     2     1     7    10     1   180.0      6.2760      2;
     2     1     8     3     1   180.0      6.2760      2;
     2     1     8     9     1   180.0      6.2760      2;
     3     5     7    10     1   180.0      8.3680      2;
     3     8     1     7     1   180.0     50.2080      2;
     4     3     5     6     1   180.0      6.2760      2;
     4     3     5     7     1   180.0      6.2760      2;
     4     3     8     9     1   180.0      6.2760      2;
     5     3     8     9     1   180.0      8.3680      2;
     5     7     1     8     1   180.0     50.2080      2;
     5     7    10    11     9     0.0      0.8075      1;
     5     7    10    11     9   180.0      0.9205      2;
     5     7    10    11     9     0.0      0.03766     3;
     6     5     3     8     1   180.0      6.2760      2;
     6     5     7    10     1   180.0      6.2760      2;
     7     1     8     9     1   180.0      8.3680      2;
     7     5     3     8     1   180.0     50.2080      2;
;    7    10    11    12     1     0.0      0.0000      0;
     8     1     7    10     1   180.0      8.3680      2;
    10    11    12    13     9     0.0    -14.6440      1;
    10    11    12    13     9   180.0      6.6944      2;
    10    11    12    13     9     0.0      6.6944      3;
    11    12    13    14     9     0.0    -14.6440      1;
    11    12    13    14     9   180.0      6.6944      2;
    11    12    13    14     9     0.0      6.6944      3;
    12    13    14    15     9     0.0    -14.6440      1;
    12    13    14    15     9   180.0      6.6944      2;
    12    13    14    15     9     0.0      6.6944      3;
    13    14    15    16     9     0.0    -14.6440      1;
    13    14    15    16     9   180.0      6.6944      2;
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```
    13    14    15    16     9     0.0      6.6944      3;
    14    15    16    17     9     0.0    -14.6440      1;
    14    15    16    17     9   180.0      6.6944      2;
    14    15    16    17     9     0.0      6.6944      3;
     1     3     8     9     4   180.0      8.3680      2;
     1     5     7    10     4   180.0      8.3680      2;
     7     5     3     6     4   180.0      4.6024      2;
     7     8     1     2     4   180.0      4.6024      2;
     8     3     5     4     4   180.0      4.6024      2;
```

c12mim.itp

```
[ moleculetype ]
; Name              nrexcl
DMI                 3

[ atoms ]
;   nr       type  resnr residue  atom   cgnr     charge       mass
     1         CR      1   DMI      Z1      1      0.0000    13.0190
     2         H5      1   DMI      Z2      2      0.1500     1.0079
     3         CW      1   DMI      Z3      3     -0.1600    13.0190
     4         H4      1   DMI      Z4      4      0.2000     1.0079
     5         CW      1   DMI      Z5      5     -0.1600    13.0190
     6         H4      1   DMI      Z6      6      0.2000     1.0079
     7         NA      1   DMI      Z7      7      0.0150    14.0067
     8         NA      1   DMI      Z8      8      0.0150    14.0067
     9        CN3      1   DMI      Z9      9      0.2600    15.0350
    10        CN2      1   DMI     Z10     10      0.2300    14.0270
    11        CTA      1   DMI     Z11     11      0.0500    14.0270
    12        CT2      1   DMI     Z12     12      0.0000    14.0270
    13        CT2      1   DMI     Z13     13      0.0000    14.0270
    14        CT2      1   DMI     Z14     14      0.0000    14.0270
    15        CT2      1   DMI     Z15     15      0.0000    14.0270
    16        CT2      1   DMI     Z16     16      0.0000    14.0270
    17        CT2      1   DMI     Z17     17      0.0000    14.0270
    18        CT2      1   DMI     Z18     18      0.0000    14.0270
    19        CT2      1   DMI     Z19     19      0.0000    14.0270
    20        CT2      1   DMI     Z20     20      0.0000    14.0270
    21        CT3      1   DMI     Z21     21      0.0000    15.0350

[ bonds ]
;  ai    aj   funct          r          k
     1     2     1     0.10700    2.8811e+05
     1     7     1     0.13250    3.4401e+05
     1     8     1     0.13250    3.4401e+05
     3     4     1     0.10700    2.8811e+05
     3     5     1     0.13430    4.0033e+05
     3     8     1     0.13780    3.4401e+05
     5     6     1     0.10700    2.8811e+05
     5     7     1     0.13780    3.4401e+05
     7    10     1     0.14920    2.1631e+05
     8     9     1     0.15000    2.1631e+05
```

```
    10    11     1     0.16100    1.6284e+05
    11    12     1     0.16100    1.6284e+05
    12    13     1     0.16100    1.6284e+05
    13    14     1     0.16100    1.6284e+05
    14    15     1     0.16100    1.6284e+05
    15    16     1     0.16100    1.6284e+05
    16    17     1     0.16100    1.6284e+05
    17    18     1     0.16100    1.6284e+05
    18    19     1     0.16100    1.6284e+05
    19    20     1     0.16100    1.6284e+05
    20    21     1     0.16100    2.1840e+05

[ pairs ]
;  ai    aj     funct
     1      6       1
     1     11       1
     1      4       1
     2      5       1
     2     10       1
     2      3       1
     2      9       1
     3     10       1
     4      6       1
     4      7       1
     4      9       1
     5      9       1
     5     11       1
     6      8       1
     6     10       1
     7      9       1
     7     12       1
     8     10       1
    10     13       1
    11     14       1
    12     15       1
    13     16       1
    14     17       1
    15     18       1
    16     19       1
    17     20       1
    18     21       1

[ angles ]
;  ai    aj    ak    funct     theta       cth
     2     1     7     1  1.2570e+02  4.2844e+02
     2     1     8     1  1.2570e+02  4.2844e+02
     7     1     8     1  1.0990e+02  6.1672e+02
     4     3     5     1  1.3070e+02  4.1840e+02
     4     3     8     1  1.2210e+02  4.2844e+02
     5     3     8     1  1.0710e+02  5.8409e+02
     3     5     6     1  1.3070e+02  4.1840e+02
     3     5     7     1  1.0710e+02  5.8409e+02
```

```
     6     5     7     1  1.2210e+02  4.2844e+02
     1     7     5     1  1.0800e+02  5.6735e+02
     1     7    10     1  1.2630e+02  5.3723e+02
     5     7    10     1  1.2570e+02  5.3723e+02
     1     8     3     1  1.0800e+02  5.6735e+02
     1     8     9     1  1.2630e+02  5.3723e+02
     3     8     9     1  1.2570e+02  5.3723e+02
     7    10    11     1  1.1220e+02  6.6944e+02
    10    11    12     1  1.0220e+02  7.8324e+02
    11    12    13     1  1.0220e+02  7.8324e+02
    12    13    14     1  1.0220e+02  7.8324e+02
    13    14    15     1  1.0220e+02  7.8324e+02
    14    15    16     1  1.0220e+02  7.8324e+02
    15    16    17     1  1.0220e+02  7.8324e+02
    16    17    18     1  1.0220e+02  7.8324e+02
    17    18    19     1  1.0220e+02  7.8324e+02
    18    19    20     1  1.0220e+02  7.8324e+02
    19    20    21     1  1.0480e+02  9.5060e+02

[ dihedrals ]
;    ai    aj    ak    al funct  theta         cth     mult
     1     7     5     3     1   180.0     50.2080      2;
     1     7     5     6     1   180.0      8.3680      2;
     1     7    10    11     9     0.0      0.0711      1;
     1     7    10    11     9   180.0     0.06276      2;
     1     7    10    11     9     0.0     -0.8870      3;
     1     8     3     4     1   180.0      8.3680      2;
     1     8     3     5     1   180.0     50.2080      2;
     2     1     7     5     1   180.0      6.2760      2;
     2     1     7    10     1   180.0      6.2760      2;
     2     1     8     3     1   180.0      6.2760      2;
     2     1     8     9     1   180.0      6.2760      2;
     3     5     7    10     1   180.0      8.3680      2;
     3     8     1     7     1   180.0     50.2080      2;
     4     3     5     6     1   180.0      6.2760      2;
     4     3     5     7     1   180.0      6.2760      2;
     4     3     8     9     1   180.0      6.2760      2;
     5     3     8     9     1   180.0      8.3680      2;
     5     7     1     8     1   180.0     50.2080      2;
     5     7    10    11     9     0.0      0.8075      1;
     5     7    10    11     9   180.0      0.9205      2;
     5     7    10    11     9     0.0      0.0377      3;
     6     5     3     8     1   180.0      6.2760      2;
     6     5     7    10     1   180.0      6.2760      2;
     7     1     8     9     1   180.0      8.3680      2;
     7     5     3     8     1   180.0     50.2080      2;
;    7    10    11    12     1     0.0      0.0000      0;
     8     1     7    10     1   180.0      8.3680      2;
    10    11    12    13     9     0.0    -14.6440      1;
    10    11    12    13     9   180.0      6.6944      2;
    10    11    12    13     9     0.0      6.6944      3;
    11    12    13    14     9     0.0    -14.6440      1;
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```
    11    12    13    14     9   180.0      6.6944      2;
    11    12    13    14     9     0.0      6.6944      3;
    12    13    14    15     9     0.0    -14.6440      1;
    12    13    14    15     9   180.0      6.6944      2;
    12    13    14    15     9     0.0      6.6944      3;
    13    14    15    16     9     0.0    -14.6440      1;
    13    14    15    16     9   180.0      6.6944      2;
    13    14    15    16     9     0.0      6.6944      3;
    14    15    16    17     9     0.0    -14.6440      1;
    14    15    16    17     9   180.0      6.6944      2;
    14    15    16    17     9     0.0      6.6944      3;
    15    16    17    18     9     0.0    -14.6440      1;
    15    16    17    18     9   180.0      6.6944      2;
    15    16    17    18     9     0.0      6.6944      3;
    16    17    18    19     9     0.0    -14.6440      1;
    16    17    18    19     9   180.0      6.6944      2;
    16    17    18    19     9     0.0      6.6944      3;
    17    18    19    20     9     0.0    -14.6440      1;
    17    18    19    20     9   180.0      6.6944      2;
    17    18    19    20     9     0.0      6.6944      3;
    18    19    20    21     9     0.0    -14.6440      1;
    18    19    20    21     9   180.0      6.6944      2;
    18    19    20    21     9     0.0      6.6944      3;
     1     3     8     9     4   180.0      8.3680      2;
     1     5     7    10     4   180.0      8.3680      2;
     8     5     3     4     4   180.0      4.6024      2;
     8     7     1     2     4   180.0      4.6024      2;
     7     3     5     6     4   180.0      4.6024      2;
```

Anions

bf4.itp

```
[ moleculetype ]
; Name              nrexcl
BF4                 3

[ atoms ]
;   nr       type  resnr residue  atom   cgnr     charge       mass
     1         BB      1    BF4     B1      1    0.428000    10.8110
     2         FF      1    BF4     F2      2   -0.307000    18.9984
     3         FF      1    BF4     F3      3   -0.307000    18.9984
     4         FF      1    BF4     F4      4   -0.307000    18.9984
     5         FF      1    BF4     F5      5   -0.307000    18.9984

[ bonds ]
;  ai    aj   funct          r         k
     1     2     1     0.13900    2.5104e+05
     1     3     1     0.13900    2.5104e+05
     1     4     1     0.13900    2.5104e+05
```

```
     1     5     1     0.13900    2.5104e+05

[ pairs ]
;  ai    aj     funct

[ angles ]
;  ai    aj    ak    funct     theta       cth
     2     1     3     1  1.0950e+02  4.1840e+02
     2     1     4     1  1.0950e+02  4.1840e+02
     2     1     5     1  1.0950e+02  4.1840e+02
     3     1     4     1  1.0950e+02  4.1840e+02
     3     1     5     1  1.0950e+02  4.1840e+02
     4     1     5     1  1.0950e+02  4.1840e+02
```

pf6.itp

```
[ moleculetype ]
; Name              nrexcl
PF6               3

[ atoms ]
;   nr       type  resnr residue  atom   cgnr     charge       mass
     1         PP      1    PF6     P1      1    0.442000    30.9738
     2         FF      1    PF6     F2      2   -0.207000    18.9984
     3         FF      1    PF6     F3      3   -0.207000    18.9984
     4         FF      1    PF6     F4      4   -0.207000    18.9984
     5         FF      1    PF6     F5      5   -0.207000    18.9984
     6         FF      1    PF6     F6      6   -0.207000    18.9984
     7         FF      1    PF6     F7      7   -0.207000    18.9984

[ bonds ]
;  ai    aj   funct          r         k
     1     2     1     0.16000    1.6736e+05
     1     3     1     0.16000    1.6736e+05
     1     4     1     0.16000    1.6736e+05
     1     5     1     0.16000    1.6736e+05
     1     6     1     0.16000    1.6736e+05
     1     7     1     0.16000    1.6736e+05

[ pairs ]
;  ai    aj     funct

[ angles ]
;  ai    aj    ak    funct     theta       cth
     2     1     3     1  9.0000e+01  8.3680e+02
     2     1     4     1  9.0000e+01  8.3680e+02
     2     1     5     1  9.0000e+01  8.3680e+02
     3     1     4     1  9.0000e+01  8.3680e+02
     3     1     5     1  9.0000e+01  8.3680e+02
     4     1     5     1  9.0000e+01  8.3680e+02
```

```
     6     1     7     1  9.0000e+01  8.3680e+02
```

ntf2.itp

```
[ moleculetype ]
; Name              nrexcl
TFN               3

[ atoms ]
;   nr       type  resnr residue  atom   cgnr     charge       mass
     1         NF      1    TFN    NN1      1     -0.2720    14.0067
     2         SF      1    TFN    SS2      2      0.6270    32.0650
     3         SF      1    TFN    SS3      3      0.6270    32.0650
     4         OF      1    TFN    OO4      4     -0.3980    15.9994
     5         OF      1    TFN    OO5      5     -0.3980    15.9994
     6         OF      1    TFN    OO6      6     -0.3980    15.9994
     7         OF      1    TFN    OO7      7     -0.3980    15.9994
     8        CF3      1    TFN    CF8      8     -0.0950    69.0059
     9        CF3      1    TFN    CF9      9     -0.0950    69.0059

[ bonds ]
;  ai    aj   funct          r          k
     1     2     1     0.15700    4.5322e+05
     1     3     1     0.15700    4.5322e+05
     2     4     1     0.14500    9.0558e+05
     2     5     1     0.14500    9.0558e+05
     2     8     1     0.24000    2.6326e+05
     3     6     1     0.14500    9.0558e+05
     3     7     1     0.14500    9.0558e+05
     3     9     1     0.24000    2.6326e+05

[ pairs ]
;  ai    aj     funct
     2      6      1
     2      7      1
     2      9      1
     3      4      1
     3      5      1
     3      8      1

[ angles ]
;  ai    aj    ak    funct     theta       cth
     2     1     3     1  1.2520e+02  1.0242e+03
     1     2     4     1  1.1270e+02  1.1749e+03
     1     2     5     1  1.1270e+02  1.1749e+03
     1     2     8     1  1.0590e+02  1.3205e+03
     4     2     5     1  1.1460e+02  1.2485e+03
     4     2     8     1  1.0320e+02  1.2803e+03
     5     2     8     1  1.0320e+02  1.2803e+03
     1     3     6     1  1.1270e+02  1.1749e+03
```

```
     1     3     7     1  1.1270e+02  1.1749e+03
     1     3     9     1  1.0590e+02  1.3205e+03
     6     3     7     1  1.1460e+02  1.2485e+03
     6     3     9     1  1.0320e+02  1.2803e+03
     7     3     9     1  1.0320e+02  1.2803e+03

[ dihedrals ]
;    ai    aj    ak    al funct  theta        cth     mult
     2     1     3     6     1     0.0      3.3472      3;
     2     1     3     7     1     0.0      3.3472      3;
     2     1     3     9     9   180.0      3.8325      1;
     2     1     3     9     9     0.0     -4.3723      2;
     2     1     3     9     9     0.0     -1.5983      3;
     3     1     2     4     1     0.0      3.3472      3;
     3     1     2     5     1     0.0      3.3472      3;
     3     1     2     8     9     0.0      3.8325      1;
     3     1     2     8     9    180.0    -4.3723      2;
     3     1     2     8     9     0.0     -1.5983      3;
```

cl.itp

```
[ moleculetype ]
; molname   nrexcl
CLA          1

[ atoms ]
; id    at type res nr  residu name at name  cg nr  charge   mass
1       CLA     1       CLA         CLA       1      -0.8       35.4530
```

Water

spc.itp

```
[ moleculetype ]
; molname        nrexcl
SOL               2

[ atoms ]
;   nr   type  resnr residue  atom   cgnr     charge       mass
#ifndef HEAVY_H
     1     OW      1    SOL     OW      1      -0.82   15.99940
     2      H      1    SOL    HW1      1       0.41    1.00800
     3      H      1    SOL    HW2      1       0.41    1.00800
#else
     1     OW      1    SOL     OW      1      -0.82    9.95140
     2      H      1    SOL    HW1      1       0.41    4.03200
     3      H      1    SOL    HW2      1       0.41    4.03200
#endif

#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
```

Lipid

popc.itp

```
[ moleculetype ]
; Name   nrexcl
 POP     3

[ atoms ]
;   nr    type   resnr  residu    atom    cgnr        charge    mass
     1     LC3        1     POP      C1       0         0.4000   15.0350
     2     LC3        1     POP      C2       0         0.4000   15.0350
     3     LC3        1     POP      C3       0         0.4000   15.0350
     4     LNL        1     POP      N4       0        -0.5000   14.0067
     5     LH2        1     POP      C5       0         0.3000   14.0270
     6     LC2        1     POP      C6       1         0.4000   14.0270
     7     LOS        1     POP      O7       1        -0.800   15.9994
     8     LP         1     POP      P8       1         1.700   30.9738
     9     LOM        1     POP      O9       1        -0.800   15.9994
    10     LOM        1     POP     O10       1        -0.800   15.9994
    11     LOS        1     POP     O11       1        -0.700   15.9994
    12     LC2        1     POP     C12       2         0.400   14.0270
    13     LH1        1     POP     C13       2         0.300   13.0190
    14     LOS        1     POP     O14       2        -0.700   15.9994
    15      LC        1     POP     C15       2         0.7000   12.0110
    16      LO        1     POP     O16       2        -0.700   15.9994
    17     LP2        1     POP     C17       3         0.0      14.0270
    18     LP2        1     POP     C18       4             0    14.0270
    19     LP2        1     POP     C19       5             0    14.0270
    20     LP2        1     POP     C20       6             0    14.0270
    21     LP2        1     POP     C21       7             0    14.0270
    22     LP2        1     POP     C22       8             0    14.0270
```

```
    23     LP2       1     POP     C23       9             0    14.0270
    24     LH1       1     POP     C24      10             0    13.0190
    25     LH1       1     POP     C25      11             0    13.0190
    26     LP2       1     POP     C26      12             0    14.0270
    27     LP2       1     POP     C27      13             0    14.0270
    28     LP2       1     POP     C28      14             0    14.0270
    29     LP2       1     POP     C29      15             0    14.0270
    30     LP2       1     POP     C30      16             0    14.0270
    31     LP2       1     POP     C31      17             0    14.0270
    32     LC2       1     POP     C32      18          0.50    14.0270
    33     LOS       1     POP     O33      18         -0.70    15.9994
    34      LC       1     POP     C34      18          0.800    12.0110
    35      LO       1     POP     O35      18         -0.60    15.9994
    36     LP2       1     POP     C36      19             0    14.0270
    37     LP2       1     POP     C37      20             0    14.0270
    38     LP2       1     POP     C38      21             0    14.0270
    39     LP2       1     POP     C39      22             0    14.0270
    40     LP2       1     POP     C40      23             0    14.0270
    41     LP2       1     POP     C41      24             0    14.0270
    42     LP2       1     POP     C42      25             0    14.0270
    43     LP2       1     POP     C43      26             0    14.0270
    44     LP2       1     POP     C44      27             0    14.0270
    45     LP2       1     POP     C45      28             0    14.0270
    46     LP2       1     POP     C46      29             0    14.0270
    47     LP2       1     POP     C47      30             0    14.0270
    48     LP2       1     POP     C48      31             0    14.0270
    49     LP2       1     POP     C49      32             0    14.0270
    50     LP3       1     POP     C50      33             0    15.0350
    51     LP2       1     POP     CA1      34             0    14.0270
    52     LP3       1     POP     CA2      35             0    15.0350

[ bonds ]
;  ai    aj funct
       4       5       1 0.14700E+00 0.37660E+06
       5       6       1 0.15300E+00 0.33470E+06
       6       7       1 0.14300E+00 0.25100E+06
       7       8       1 0.16100E+00 0.25100E+06
       8       9       1 0.14800E+00 0.37660E+06
       8      10       1 0.14800E+00 0.37660E+06
       8      11       1 0.16100E+00 0.25100E+06
      11      12       1 0.14300E+00 0.25100E+06
      12      13       1 0.15300E+00 0.33470E+06
      13      14       1 0.14350E+00 0.25100E+06
      13      32       1 0.15300E+00 0.33470E+06
      14      15       1 0.13600E+00 0.37660E+06
      15      16       1 0.12300E+00 0.50210E+06
      15      17       1 0.15300E+00 0.33470E+06
      17      18       1 0.15300E+00 0.33470E+06
      18      19       1 0.15300E+00 0.33470E+06
      19      20       1 0.15300E+00 0.33470E+06
      20      21       1 0.15300E+00 0.33470E+06
      21      22       1 0.15300E+00 0.33470E+06
```

```
      22      23       1 0.15300E+00 0.33470E+06
      23      24       1 0.15300E+00 0.33470E+06
      24      25       1 0.13900E+00 0.41840E+06
      25      26       1 0.15300E+00 0.33470E+06
      26      27       1 0.15300E+00 0.33470E+06
      27      28       1 0.15300E+00 0.33470E+06
      28      29       1 0.15300E+00 0.33470E+06
      29      30       1 0.15300E+00 0.33470E+06
      30      31       1 0.15300E+00 0.33470E+06
      31      51       1 0.15300E+00 0.33470E+06
      51      52       1 0.15300E+00 0.33470E+06
      32      33       1 0.14300E+00 0.25100E+06
      33      34       1 0.13600E+00 0.37660E+06
      34      35       1 0.12300E+00 0.50210E+06
      34      36       1 0.15300E+00 0.33470E+06
      36      37       1 0.15300E+00 0.33470E+06
      37      38       1 0.15300E+00 0.33470E+06
      38      39       1 0.15300E+00 0.33470E+06
      39      40       1 0.15300E+00 0.33470E+06
      40      41       1 0.15300E+00 0.33470E+06
      41      42       1 0.15300E+00 0.33470E+06
      42      43       1 0.15300E+00 0.33470E+06
      43      44       1 0.15300E+00 0.33470E+06
      44      45       1 0.15300E+00 0.33470E+06
      45      46       1 0.15300E+00 0.33470E+06
      46      47       1 0.15300E+00 0.33470E+06
      47      48       1 0.15300E+00 0.33470E+06
      48      49       1 0.15300E+00 0.33470E+06
      49      50       1 0.15300E+00 0.33470E+06
       1       4       1 0.14700E+00 0.37450E+06
       2       4       1 0.14700E+00 0.37450E+06
       3       4       1 0.14700E+00 0.37450E+06

[ pairs ]
;  ai    aj funct
    1     6     1
    2     6     1
    3     6     1
    4     7     1
    5     8     1
    6     9     1
    6    10     1
    6    11     1
    7    12     1
    8    13     1
    9    12     1
   10    12     1
   11    14     1
   11    32     1
   12    15     1
   12    33     1
   13    16     1
```

```
   13    17     1
   13    34     1
   14    18     1
   14    33     1
   15    19     1
   15    32     1
   16    18     1
   22    25     1    ; pair around double bond
   24    27     1    ; pair around double bond
   32    35     1
   32    36     1
   33    37     1
   34    38     1
   35    37     1
;;list pairs twice to account for 1.0 fudge QQ for lipid
    1     6     1
    2     6     1
    3     6     1
    4     7     1
    5     8     1
    6     9     1
    6    10     1
    6    11     1
    7    12     1
    8    13     1
    9    12     1
   10    12     1
   11    14     1
   11    32     1
   12    15     1
   12    33     1
   13    16     1
   13    17     1
   13    34     1
   14    18     1
   14    33     1
   15    19     1
   15    32     1
   16    18     1
   22    25     1    ; pair around double bond
   24    27     1    ; pair around double bond
   32    35     1
   32    36     1
   33    37     1
   34    38     1
   35    37     1

[ angles ]
;  ai    aj    ak funct
       4       5       6       1 0.10950E+03 0.46020E+03
       5       6       7       1 0.10950E+03 0.46020E+03
       6       7       8       1 0.12000E+03 0.39750E+03
```

```
     7       8       9       1 0.10960E+03 0.39750E+03
     7       8      10       1 0.10960E+03 0.39750E+03
     7       8      11       1 0.10300E+03 0.39750E+03
     8      11      12       1 0.12000E+03 0.39750E+03
     9       8      10       1 0.12000E+03 0.58580E+03
     9       8      11       1 0.10960E+03 0.39750E+03
    10       8      11       1 0.10960E+03 0.39750E+03
    11      12      13       1 0.11100E+03 0.46020E+03
    12      13      14       1 0.10950E+03 0.46020E+03
    12      13      32       1 0.10950E+03 0.46020E+03
    13      14      15       1 0.12000E+03 0.41840E+03
    13      32      33       1 0.11100E+03 0.46020E+03
    14      13      32       1 0.10950E+03 0.46020E+03
    14      15      16       1 0.12400E+03 0.50210E+03
    14      15      17       1 0.11500E+03 0.50210E+03
    15      17      18       1 0.11100E+03 0.46020E+03
    16      15      17       1 0.12100E+03 0.50210E+03
    17      18      19       1 0.11100E+03 0.46020E+03
    18      19      20       1 0.11100E+03 0.46020E+03
    19      20      21       1 0.11100E+03 0.46020E+03
    20      21      22       1 0.11100E+03 0.46020E+03
    21      22      23       1 0.11100E+03 0.46020E+03
    22      23      24       1 0.11100E+03 0.46020E+03
23    24    25     1    120.000     502.080  ; cis thingies
24    25    26     1    120.000     502.080  ; cis thingies
    25      26      27       1 0.11100E+03 0.46020E+03
    26      27      28       1 0.11100E+03 0.46020E+03
    27      28      29       1 0.11100E+03 0.46020E+03
    28      29      30       1 0.11100E+03 0.46020E+03
    29      30      31       1 0.11100E+03 0.46020E+03
30    31    51     1 0.11100E+03 0.46020E+03
31    51    52     1 0.11100E+03 0.46020E+03
    32      33      34       1 0.12000E+03 0.41840E+03
    33      34      35       1 0.12400E+03 0.50210E+03
    33      34      36       1 0.11500E+03 0.50210E+03
    34      36      37       1 0.11100E+03 0.46020E+03
    35      34      36       1 0.12100E+03 0.50210E+03
    36      37      38       1 0.11100E+03 0.46020E+03
    37      38      39       1 0.11100E+03 0.46020E+03
    38      39      40       1 0.11100E+03 0.46020E+03
    39      40      41       1 0.11100E+03 0.46020E+03
    40      41      42       1 0.11100E+03 0.46020E+03
    41      42      43       1 0.11100E+03 0.46020E+03
    42      43      44       1 0.11100E+03 0.46020E+03
    43      44      45       1 0.11100E+03 0.46020E+03
    44      45      46       1 0.11100E+03 0.46020E+03
    45      46      47       1 0.11100E+03 0.46020E+03
    46      47      48       1 0.11100E+03 0.46020E+03
    47      48      49       1 0.11100E+03 0.46020E+03
    48      49      50       1 0.11100E+03 0.46020E+03
     1       4       2       1 0.10950E+03 0.33470E+03
     2       4       3       1 0.10950E+03 0.33470E+03
```

```
       3       4       1       1 0.10950E+03 0.33470E+03
       1       4       5       1 0.10950E+03 0.37660E+03
       2       4       5       1 0.10950E+03 0.37660E+03
       3       4       5       1 0.10950E+03 0.37660E+03

[ dihedrals ]
;  ai    aj    ak    al funct   phi0     cp     mult
    1     4     5     6     1    0.0     3.76   3
    4     5     6     7     1    0.0     5.85   3
    5     6     7     8     1    0.0     3.76   3
    6     7     8    11     1    0.0     1.05   3
    6     7     8    11     1    0.0     3.14   2
    7     8    11    12     1    0.0     1.05   3
    7     8    11    12     1    0.0     3.14   2
    8    11    12    13     1    0.0     3.76   3
   11    12    13    14     1    0.0     2.09   2
   11    12    13    32     1    0.0     5.85   3
   11    12    13    32     1    0.0     0.42   2
   12    13    32    33     1    0.0     5.85   3
   12    13    32    33     1    0.0     0.42   2
   12    13    14    15     1    0.0     3.77   3
   13    32    33    34     1    0.0     3.76   3
   13    14    15    17     1    180.0  16.74   2
   14    13    32    33     1    0.0     2.09   2
   14    15    17    18     1    0.0     0.42   6
   15    17    18    19     1    0.0     5.86   3
   17    18    19    20     3
   18    19    20    21     3
   19    20    21    22     3
   20    21    22    23     3
   21    22    23    24     3
   22    23    24    25     1 0.000       5.858      3
;   23    24    25    26     1
   24    25    26    27     1 0.000       5.858      3
   25    26    27    28     3
   26    27    28    29     3
   27    28    29    30     3
   28    29    30    31     3
   29    30    31    51     3
   30    31    51    52     3
   13    32    33    34     1    0.0     3.76    3
   32    33    34    36     1    180.0   16.74   2
   33    34    36    37     1    0.0     0.42    6
   34    36    37    38     1    0.0     5.86    3
   36    37    38    39     3
   37    38    39    40     3
   38    39    40    41     3
   39    40    41    42     3
   40    41    42    43     3
   41    42    43    44     3
   42    43    44    45     3
   43    44    45    46     3
```

```
   44    45    46    47     3
   45    46    47    48     3
   46    47    48    49     3
   47    48    49    50     3

[ dihedrals ]
;  ai    aj    ak    al funct
      13      14      32      12       2 35.264      0.33470E+03
      15      14      17      16       2 0.00000E+00 0.16740E+03
      34      33      36      35       2 0.00000E+00 0.16740E+03
      23      24      25      26       2 0.000     167.360

#ifdef POSRES_LIPID
#include "lipid_posre.itp"
#endif
```

Nonbonded Interactions

```
[ defaults ]
; nbfunc        comb-rule        gen-pairs        fudgeLJ        fudgeQQ
  1               1                no               0.5        0.5

[ atomtypes ]
   LO    8     15.9994    0.000  A 2.36400e-03 1.59000e-06 ;carbonyl O, OPLS
  LOM    8     15.9994    0.000  A 2.36400e-03 1.59000e-06 ;carboxyl O, OPLS
  LNL    7     14.0067    0.000  A 3.35300e-03 3.95100e-06 ;Nitrogen, OPLS
   LC    6     12.0110    0.000  A 4.88800e-03 1.35900e-05 ;Carbonyl C, OPLS
  LH1    6     13.0190    0.000  A 4.03100e-03 1.21400e-05 ;CH1, OPLS
  LH2    6     14.0270    0.000  A 7.00200e-03 2.48300e-05 ;CH2, OPLS
   LP    15    30.9738    0.000  A 9.16000e-03 2.50700e-05 ;phosphor, OPLS
  LOS    8     15.9994    0.000  A 2.56300e-03 1.86800e-06 ;ester oxygen, OPLS
  LP2    6     14.0270    0.000  A 5.87400e-03 2.26500e-05 ;RB CH2, Bergers LJ
  LP3    6     15.0350    0.000  A 8.77700e-03 3.38500e-05 ;RB CH3, Bergers LJ
  LC3    6     15.0350    0.000  A 9.35700e-03 3.60900e-05 ;CH3, OPLS
  LC2    6     14.0270    0.000  A 5.94700e-03 1.79000e-05 ;CH2, OPLS
   CR      6 13.0190  0.0000  A  2.223430e-03   3.43477e-06
   H5      1  1.0079  0.0000  A  1.887870e-06   7.09856e-12
   CW      6 13.0190  0.0000  A  2.223430e-03   3.43477e-06
   H4      1  1.0079  0.0000  A  8.550650e-06   1.45621e-10
   NA      7 14.0067  0.0000  A  3.352750e-03   3.95094e-06
  CN3      6 15.0350  0.0000  A  9.772510e-03   3.00336e-05
  CN2      6 14.0270  0.0000  A  7.407710e-03   2.30902e-05
  CTA      6 14.0270  0.0000  A  8.416010e-03   3.18206e-05
  CT2      6 14.0270  0.0000  A  8.416010e-03   3.18206e-05
  CT3      6 15.0350  0.0000  A  1.092820e-02   3.85719e-05
   NF      7 14.0067  0.0000  A  8.013260e+02   9.44298e+05
   SF     16 32.0650  0.0000  A  2.049400e+03   4.20003e+06
   OF      8 15.9994  0.0000  A  5.649750e+02   3.79997e+05
  CF3      6 69.0059  0.0000  A  5.119070e+03   4.09451e+07
  CLA   17      0.000      0.000     A  6.89232E-03  1.89229E-05
   PP     15 30.9738  0.442000  A  1.073170e-02   3.44078e-05
   FF      9 18.9984 -0.207000  A  9.534550e-04   8.76106e-07
```

```
   BB      1       0       0  A             0             0

[ nonbond_params ]
   LO    LO     1 2.36400e-03  1.59000e-06
   LO   LOM     1 2.36400e-03  1.59000e-06
   LO   LNL     1 2.81600e-03  2.50600e-06
   LO    LC     1 3.39900e-03  4.64800e-06
   LO   LH1     1 3.08700e-03  4.39300e-06
   LO   LH2     1 4.06900e-03  6.28300e-06
   LO    LP     1 4.65300e-03  6.31300e-06
   LO   LOS     1 2.46100e-03  1.72300e-06
   LO   LP2     1 3.72700e-03  6.00000e-06
   LO   LP3     1 4.55500e-03  7.33500e-06
   LO   LC3     1 4.70300e-03  7.57400e-06
   LO   LC2     1 3.74900e-03  5.33500e-06
  LOM   LOM     1 2.36400e-03  1.59000e-06
  LOM   LNL     1 2.81600e-03  2.50600e-06
  LOM    LC     1 3.39900e-03  4.64800e-06
  LOM   LH1     1 3.08700e-03  4.39300e-06
  LOM   LH2     1 4.06900e-03  6.28300e-06
  LOM    LP     1 4.65300e-03  6.31300e-06
  LOM   LOS     1 2.46100e-03  1.72300e-06
  LOM   LP2     1 3.72700e-03  6.00000e-06
  LOM   LP3     1 4.55500e-03  7.33500e-06
  LOM   LC3     1 4.70300e-03  7.57400e-06
  LOM   LC2     1 3.74900e-03  5.33500e-06
  LNL   LNL     1 3.35300e-03  3.95100e-06
  LNL    LC     1 4.04900e-03  7.32800e-06
  LNL   LH1     1 3.67700e-03  6.92500e-06
  LNL   LH2     1 4.84600e-03  9.90500e-06
  LNL    LP     1 5.54200e-03  9.95300e-06
  LNL   LOS     1 2.93200e-03  2.71700e-06
  LNL   LP2     1 4.43800e-03  9.46000e-06
  LNL   LP3     1 5.42500e-03  1.15600e-05
  LNL   LC3     1 5.60100e-03  1.19400e-05
  LNL   LC2     1 4.46600e-03  8.41100e-06
   LC    LC     1 4.88800e-03  1.35900e-05
   LC   LH1     1 4.43900e-03  1.28400e-05
   LC   LH2     1 5.85100e-03  1.83700e-05
   LC    LP     1 6.69100e-03  1.84600e-05
   LC   LOS     1 3.53900e-03  5.03800e-06
   LC   LP2     1 5.35900e-03  1.75400e-05
   LC   LP3     1 6.55000e-03  2.14500e-05
   LC   LC3     1 6.76300e-03  2.21500e-05
   LC   LC2     1 5.39100e-03  1.56000e-05
  LH1   LH1     1 4.03100e-03  1.21400e-05
  LH1   LH2     1 5.31300e-03  1.73600e-05
  LH1    LP     1 6.07700e-03  1.74400e-05
  LH1   LOS     1 3.21400e-03  4.76100e-06
  LH1   LP2     1 4.86600e-03  1.65800e-05
  LH1   LP3     1 5.94800e-03  2.02700e-05
  LH1   LC3     1 6.14200e-03  2.09300e-05
```

```
  LH1   LC2     1 4.89600e-03  1.47400e-05
  LH2   LH2     1 7.00200e-03  2.48300e-05
  LH2    LP     1 8.00900e-03  2.49500e-05
  LH2   LOS     1 4.23600e-03  6.81000e-06
  LH2   LP2     1 6.41400e-03  2.37100e-05
  LH2   LP3     1 7.83900e-03  2.89900e-05
  LH2   LC3     1 8.09500e-03  2.99300e-05
  LH2   LC2     1 6.45300e-03  2.10800e-05
   LP    LP     1 9.16000e-03  2.50700e-05
   LP   LOS     1 4.84500e-03  6.84200e-06
   LP   LP2     1 7.33500e-03  2.38300e-05
   LP   LP3     1 8.96600e-03  2.91300e-05
   LP   LC3     1 9.25800e-03  3.00800e-05
   LP   LC2     1 7.38100e-03  2.11900e-05
  LOS   LOS     1 2.56300e-03  1.86800e-06
  LOS   LP2     1 3.88000e-03  6.50400e-06
  LOS   LP3     1 4.74300e-03  7.95100e-06
  LOS   LC3     1 4.89700e-03  8.21000e-06
  LOS   LC2     1 3.90400e-03  5.78200e-06
  LP2   LP2     1 5.87400e-03  2.26500e-05
  LP2   LP3     1 7.18000e-03  2.76900e-05
  LP2   LC3     1 7.41400e-03  2.85900e-05
  LP2   LC2     1 5.91000e-03  2.01400e-05
  LP3   LP3     1 8.77700e-03  3.38500e-05
  LP3   LC3     1 9.06200e-03  3.49500e-05
  LP3   LC2     1 7.22400e-03  2.46200e-05
  LC3   LC3     1 9.35700e-03  3.60900e-05
  LC3   LC2     1 7.45900e-03  2.54200e-05
  LC2   LC2     1 5.94700e-03  1.79000e-05
;; lipid-SPC/SPCE interactions
   LO    OW    1 2.50200e-03  2.06700e-06
  LOM    OW    1 2.50200e-03  2.06700e-06
  LNL    OW    1 2.98000e-03  3.25900e-06
   LC    OW    1 3.59800e-03  6.04400e-06
  LH1    OW    1 3.26800e-03  5.71200e-06
  LH2    OW    1 4.30700e-03  8.17000e-06
   LP    OW    1 4.92600e-03  8.21000e-06
  LOS    OW    1 2.60500e-03  2.24100e-06
  LP2    OW    1 3.94400e-03  7.80300e-06
  LP3    OW    1 4.82100e-03  9.53900e-06
  LC3    OW    1 4.97800e-03  9.85000e-06
  LC2    OW    1 3.96900e-03  6.93800e-06
  LNL     H    1 0.000000e+00 0.000000e+00
  LOS     H    1 0.000000e+00 0.000000e+00
  LOM     H    1 0.000000e+00 0.000000e+00
   LO     H    1 0.000000e+00 0.000000e+00
   LP     H    1 0.000000e+00 0.000000e+00
   LC     H    1 0.000000e+00 0.000000e+00
  LH1     H    1 0.000000e+00 0.000000e+00
  LC2     H    1 0.000000e+00 0.000000e+00
  LH2     H    1 0.000000e+00 0.000000e+00
  LP2     H    1 0.000000e+00 0.000000e+00
```

```
  LP3     H    1 0.000000e+00 0.000000e+00
  LC3     H    1 0.000000e+00 0.000000e+00
;;IL-IL nonbond interactions
    NA    NA     1  3.3527e-03  3.9509e-06
    NA    CR     1  2.7345e-03  3.6951e-06
    NA    CW     1  2.7345e-03  3.6951e-06
    NA    H5     1  1.5445e-04  1.9960e-08
    NA    H4     1  2.4426e-04  4.9920e-08
    NA   CN3     1  5.8346e-03  1.1318e-05
    NA   CN2     1  5.0827e-03  9.9350e-06
    NA   CTA     1  5.4643e-03  1.1865e-05
    NA   CT2     1  5.4643e-03  1.1865e-05
    NA   CT3     1  6.2065e-03  1.2979e-05
    NA   CLA     1  4.8792e-03  8.9080e-06
    NA   CF3     1  9.1437e-03  3.0291e-05
    NA    NF     1  3.3528e-03  3.9510e-06
    NA    SF     1  5.3961e-03  8.4394e-06
    NA    OF     1  2.8336e-03  2.5393e-06
    NA    PP     1  5.6244e-03  1.0251e-05
    NA    FF     1  1.7902e-03  1.8653e-06
    NA    BB     1  3.3912e-03  5.3790e-06
    CR    CR     1  2.2234e-03  3.4348e-06
    CR    CW     1  2.2234e-03  3.4348e-06
    CR    H5     1  1.3376e-04  2.1046e-08
    CR    H4     1  2.0854e-04  5.1157e-08
    CR   CN3     1  4.7075e-03  1.0359e-05
    CR   CN2     1  4.1002e-03  9.0902e-06
    CR   CTA     1  4.3985e-03  1.0809e-05
    CR   CT2     1  4.3985e-03  1.0809e-05
    CR   CT3     1  4.9999e-03  1.1842e-05
    CR   CLA     1  3.9417e-03  8.1738e-06
    CR   CF3     1  7.2993e-03  2.7140e-05
    CR    NF     1  2.7345e-03  3.6951e-06
    CR    SF     1  4.3736e-03  7.7950e-06
    CR    OF     1  2.3258e-03  2.4051e-06
    CR    PP     1  4.5439e-03  9.4066e-06
    CR    FF     1  1.4642e-03  1.7543e-06
    CR    BB     1  2.7478e-03  4.9653e-06
    CW    CW     1  2.2234e-03  3.4348e-06
    CW    H5     1  1.3376e-04  2.1046e-08
    CW    H4     1  2.0854e-04  5.1157e-08
    CW   CN3     1  4.7075e-03  1.0359e-05
    CW   CN2     1  4.1002e-03  9.0902e-06
    CW   CTA     1  4.3985e-03  1.0809e-05
    CW   CT2     1  4.3985e-03  1.0809e-05
    CW   CT3     1  4.9999e-03  1.1842e-05
    CW   CLA     1  3.9417e-03  8.1738e-06
    CW   CF3     1  7.2993e-03  2.7140e-05
    CW    NF     1  2.7345e-03  3.6951e-06
    CW    SF     1  4.3736e-03  7.7950e-06
    CW    OF     1  2.3258e-03  2.4051e-06
    CW    PP     1  4.5439e-03  9.4066e-06
```

CW	FF	1	1.4642e-03	1.7543e-06
CW	BB	1	2.7478e-03	4.9653e-06
H5	H5	1	1.8879e-06	7.0986e-12
H5	H4	1	4.2129e-06	3.5349e-11
H5	CN3	1	3.3137e-04	8.6903e-08
H5	CN2	1	2.8954e-04	7.6747e-08
H5	CTA	1	3.2432e-04	9.9495e-08
H5	CT2	1	3.2432e-04	9.9495e-08
H5	CT3	1	3.6304e-04	1.0571e-07
H5	CLA	1	2.7049e-04	6.5172e-08
H5	CF3	1	6.3387e-04	3.4653e-07
H5	NF	1	1.5445e-04	1.9960e-08
H5	SF	1	2.8081e-04	5.4406e-08
H5	OF	1	1.1507e-04	9.9683e-09
H5	PP	1	3.1159e-04	7.4893e-08
H5	FF	1	7.8007e-05	8.4306e-09
H5	BB	1	1.7751e-04	3.5085e-08
H4	H4	1	8.5506e-06	1.4562e-10
H4	CN3	1	4.9884e-04	1.9694e-07
H4	CN2	1	4.3557e-04	1.7368e-07
H4	CTA	1	4.8327e-04	2.2092e-07
H4	CT2	1	4.8327e-04	2.2092e-07
H4	CT3	1	5.4279e-04	2.3630e-07
H4	CLA	1	4.0950e-04	1.4936e-07
H4	CF3	1	9.1156e-04	7.1666e-07
H4	NF	1	2.4427e-04	4.9921e-08
H4	SF	1	4.3146e-04	1.2844e-07
H4	OF	1	1.8759e-04	2.6491e-08
H4	PP	1	4.7179e-04	1.7170e-07
H4	FF	1	1.2502e-04	2.1655e-08
H4	BB	1	2.7237e-04	8.2598e-08
CN3	CN3	1	9.7725e-03	3.0034e-05
CN3	CN2	1	8.5084e-03	2.6334e-05
CN3	CTA	1	9.0770e-03	3.0970e-05
CN3	CT2	1	9.0770e-03	3.0970e-05
CN3	CT3	1	1.0338e-02	3.4063e-05
CN3	CLA	1	8.2092e-03	2.3852e-05
CN3	CF3	1	1.4745e-02	7.4512e-05
CN3	NF	1	5.8346e-03	1.1318e-05
CN3	SF	1	9.1854e-03	2.3131e-05
CN3	OF	1	5.0424e-03	7.6057e-06
CN3	PP	1	9.4641e-03	2.7455e-05
CN3	FF	1	3.1464e-03	5.4502e-06
CN3	BB	1	5.7664e-03	1.4711e-05
CN2	CN2	1	7.4077e-03	2.3090e-05
CN2	CTA	1	7.9019e-03	2.7148e-05
CN2	CT2	1	7.9019e-03	2.7148e-05
CN2	CT3	1	9.0003e-03	2.9863e-05
CN2	CLA	1	7.1478e-03	2.0917e-05
CN2	CF3	1	1.2831e-02	6.5261e-05
CN2	NF	1	5.0828e-03	9.9351e-06
CN2	SF	1	7.9991e-03	2.0292e-05

```
CN2     OF      1   4.3940e-03   6.6808e-06
CN2     PP      1   8.2404e-03   2.4076e-05
CN2     FF      1   2.7414e-03   4.7857e-06
CN2     BB      1   5.0216e-03   1.2905e-05
CTA    CTA      1   8.4160e-03   3.1821e-05
CTA    CT2      1   8.4160e-03   3.1821e-05
CTA    CT3      1   9.5911e-03   3.5041e-05
CTA    CLA      1   7.6324e-03   2.4643e-05
CTA    CF3      1   1.3583e-02   7.5577e-05
CTA     NF      1   5.4643e-03   1.1865e-05
CTA     SF      1   8.5616e-03   2.4019e-05
CTA     OF      1   4.7450e-03   8.0499e-06
CTA     PP      1   8.7994e-03   2.8367e-05
CTA     FF      1   2.9530e-03   5.7380e-06
CTA     BB      1   5.3736e-03   1.5269e-05
CT2    CT2      1   8.4160e-03   3.1821e-05
CT2    CT3      1   9.5911e-03   3.5041e-05
CT2    CLA      1   7.6324e-03   2.4643e-05
CT2    CF3      1   1.3583e-02   7.5577e-05
CT2     NF      1   5.4643e-03   1.1865e-05
CT2     SF      1   8.5616e-03   2.4019e-05
CT2     OF      1   4.7450e-03   8.0499e-06
CT2     PP      1   8.7994e-03   2.8367e-05
CT2     FF      1   2.9530e-03   5.7380e-06
CT2     BB      1   5.3736e-03   1.5269e-05
CT3    CT3      1   1.0928e-02   3.8572e-05
CT3    CLA      1   8.6901e-03   2.7088e-05
CT3    CF3      1   1.5513e-02   8.3583e-05
CT3     NF      1   6.2066e-03   1.2979e-05
CT3     SF      1   9.7399e-03   2.6357e-05
CT3     OF      1   5.3810e-03   8.7778e-06
CT3     PP      1   1.0019e-02   3.1180e-05
CT3     FF      1   3.3518e-03   6.2679e-06
CT3     BB      1   6.1136e-03   1.6758e-05
CLA    CLA      1   6.8923e-03   1.8923e-05
CLA    CF3      1   1.2442e-02   5.9709e-05
CLA     NF      1   4.8793e-03   8.9081e-06
CLA     SF      1   7.7013e-03   1.8301e-05
CLA     OF      1   4.2058e-03   5.9551e-06
CLA     PP      1   7.9458e-03   2.1780e-05
CLA     FF      1   2.6282e-03   4.2798e-06
CLA     BB      1   4.8354e-03   1.1642e-05
CF3    CF3      1   2.1417e-02   1.7130e-04
CF3     NF      1   9.1438e-03   3.0292e-05
CF3     SF      1   1.4084e-02   5.9264e-05
CF3     OF      1   8.0770e-03   2.1267e-05
CF3     PP      1   1.4346e-02   6.8745e-05
CF3     FF      1   4.9793e-03   1.4874e-05
CF3     BB      1   8.8324e-03   3.7611e-05
 NF     NF      1   3.3528e-03   3.9511e-06
 NF     SF      1   5.3962e-03   8.4395e-06
 NF     OF      1   2.8337e-03   2.5393e-06
```

```
    NF    PP     1  5.6245e-03  1.0251e-05
    NF    FF     1  1.7903e-03  1.8653e-06
    NF    BB     1  3.3913e-03  5.3791e-06
    SF    SF     1  8.5747e-03  1.7573e-05
    SF    OF     1  4.6198e-03  5.5658e-06
    SF    PP     1  8.8781e-03  2.1062e-05
    SF    FF     1  2.8979e-03  4.0303e-06
    SF    BB     1  5.3855e-03  1.1187e-05
    OF    OF     1  2.3637e-03  1.5898e-06
    OF    PP     1  4.8477e-03  6.8518e-06
    OF    FF     1  1.5043e-03  1.1850e-06
    OF    BB     1  2.9052e-03  3.5519e-06
    PP    PP     1  9.1603e-03  2.5069e-05
    PP    FF     1  3.0295e-03  4.9246e-06
    PP    BB     1  5.5743e-03  1.3399e-05
    FF    FF     1  9.5345e-04  8.7611e-07
    FF    BB     1  1.8217e-03  2.5702e-06
    BB    BB     1  3.3824e-03  7.1206e-06
;;IL-lipid nonbond interactions
    NA    LO     1  2.8338e-03  2.5395e-06
    NA   LOM     1  2.8338e-03  2.5395e-06
    NA   LNL     1  3.3530e-03  3.9513e-06
    NA    LC     1  4.1112e-03  7.5575e-06
    NA   LH1     1  3.7437e-03  7.1821e-06
    NA   LH2     1  4.9687e-03  1.0417e-05
    NA    LP     1  5.6240e-03  1.0250e-05
    NA   LOS     1  2.9458e-03  2.7435e-06
    NA   LP2     1  4.5694e-03  1.0030e-05
    NA   LP3     1  5.5851e-03  1.2259e-05
    NA   LC3     1  5.7667e-03  1.2658e-05
    NA   LC2     1  4.5484e-03  8.7259e-06
    CR    LO     1  2.3259e-03  2.4052e-06
    CR   LOM     1  2.3259e-03  2.4052e-06
    CR   LNL     1  2.7347e-03  3.6954e-06
    CR    LC     1  3.3208e-03  6.9326e-06
    CR   LH1     1  3.0212e-03  6.5765e-06
    CR   LH2     1  4.0025e-03  9.5033e-06
    CR    LP     1  4.5436e-03  9.4061e-06
    CR   LOS     1  2.4156e-03  2.5937e-06
    CR   LP2     1  3.6774e-03  9.1333e-06
    CR   LP3     1  4.4948e-03  1.1163e-05
    CR   LC3     1  4.6410e-03  1.1526e-05
    CR   LC2     1  3.6706e-03  7.9901e-06
    CW    LO     1  2.3259e-03  2.4052e-06
    CW   LOM     1  2.3259e-03  2.4052e-06
    CW   LNL     1  2.7347e-03  3.6954e-06
    CW    LC     1  3.3208e-03  6.9326e-06
    CW   LH1     1  3.0212e-03  6.5765e-06
    CW   LH2     1  4.0025e-03  9.5033e-06
    CW    LP     1  4.5436e-03  9.4061e-06
    CW   LOS     1  2.4156e-03  2.5937e-06
    CW   LP2     1  3.6774e-03  9.1333e-06
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CW	LP3	1	4.4948e-03	1.1163e-05
CW	LC3	1	4.6410e-03	1.1526e-05
CW	LC2	1	3.6706e-03	7.9901e-06
H5	LO	1	1.1508e-04	9.9689e-09
H5	LOM	1	1.1508e-04	9.9689e-09
H5	LNL	1	1.5447e-04	1.9961e-08
H5	LC	1	2.2855e-04	5.5597e-08
H5	LH1	1	2.1169e-04	5.4666e-08
H5	LH2	1	2.9092e-04	8.5007e-08
H5	LP	1	3.1157e-04	7.4888e-08
H5	LOS	1	1.2183e-04	1.1170e-08
H5	LP2	1	2.7234e-04	8.4812e-08
H5	LP3	1	3.3287e-04	1.0366e-07
H5	LC3	1	3.4370e-04	1.0703e-07
H5	LC2	1	2.5719e-04	6.6416e-08
H4	LO	1	1.8760e-04	2.6493e-08
H4	LOM	1	1.8760e-04	2.6493e-08
H4	LNL	1	2.4428e-04	4.9924e-08
H4	LC	1	3.4577e-04	1.2726e-07
H4	LH1	1	3.1900e-04	1.2414e-07
H4	LH2	1	4.3487e-04	1.8994e-07
H4	LP	1	4.7176e-04	1.7169e-07
H4	LOS	1	1.9773e-04	2.9424e-08
H4	LP2	1	4.0542e-04	1.8795e-07
H4	LP3	1	4.9554e-04	2.2973e-07
H4	LC3	1	5.1165e-04	2.3720e-07
H4	LC2	1	3.8757e-04	1.5082e-07
CN3	LO	1	5.0427e-03	7.6062e-06
CN3	LOM	1	5.0427e-03	7.6062e-06
CN3	LNL	1	5.8351e-03	1.1319e-05
CN3	LC	1	6.9135e-03	2.0215e-05
CN3	LH1	1	6.2755e-03	1.9090e-05
CN3	LH2	1	8.2750e-03	2.7329e-05
CN3	LP	1	9.4636e-03	2.7453e-05
CN3	LOS	1	5.2252e-03	8.1649e-06
CN3	LP2	1	7.5846e-03	2.6139e-05
CN3	LP3	1	9.2705e-03	3.1949e-05
CN3	LC3	1	9.5719e-03	3.2988e-05
CN3	LC2	1	7.6244e-03	2.3193e-05
CN2	LO	1	4.3943e-03	6.6812e-06
CN2	LOM	1	4.3943e-03	6.6812e-06
CN2	LNL	1	5.0831e-03	9.9358e-06
CN2	LC	1	6.0195e-03	1.7727e-05
CN2	LH1	1	5.4638e-03	1.6739e-05
CN2	LH2	1	7.2040e-03	2.3958e-05
CN2	LP	1	8.2400e-03	2.4075e-05
CN2	LOS	1	4.5531e-03	7.1713e-06
CN2	LP2	1	6.6026e-03	2.2913e-05
CN2	LP3	1	8.0702e-03	2.8006e-05
CN2	LC3	1	8.3326e-03	2.8917e-05
CN2	LC2	1	6.6382e-03	2.0337e-05
CTA	LO	1	4.7452e-03	8.0504e-06

CTA	LOM	1	4.7452e-03	8.0504e-06
CTA	LNL	1	5.4647e-03	1.1866e-05
CTA	LC	1	6.4270e-03	2.0881e-05
CTA	LH1	1	5.8300e-03	1.9692e-05
CTA	LH2	1	7.6766e-03	2.8111e-05
CTA	LP	1	8.7989e-03	2.8365e-05
CTA	LOS	1	4.9137e-03	8.6300e-06
CTA	LP2	1	7.0311e-03	2.6848e-05
CTA	LP3	1	8.5939e-03	3.2816e-05
CTA	LC3	1	8.8733e-03	3.3883e-05
CTA	LC2	1	7.0831e-03	2.3925e-05
CT2	LO	1	4.7452e-03	8.0504e-06
CT2	LOM	1	4.7452e-03	8.0504e-06
CT2	LNL	1	5.4647e-03	1.1866e-05
CT2	LC	1	6.4270e-03	2.0881e-05
CT2	LH1	1	5.8300e-03	1.9692e-05
CT2	LH2	1	7.6766e-03	2.8111e-05
CT2	LP	1	8.7989e-03	2.8365e-05
CT2	LOS	1	4.9137e-03	8.6300e-06
CT2	LP2	1	7.0311e-03	2.6848e-05
CT2	LP3	1	8.5939e-03	3.2816e-05
CT2	LC3	1	8.8733e-03	3.3883e-05
CT2	LC2	1	7.0831e-03	2.3925e-05
CT3	LO	1	5.3813e-03	8.7783e-06
CT3	LOM	1	5.3813e-03	8.7783e-06
CT3	LNL	1	6.2070e-03	1.2980e-05
CT3	LC	1	7.3180e-03	2.2954e-05
CT3	LH1	1	6.6397e-03	2.1656e-05
CT3	LH2	1	8.7469e-03	3.0944e-05
CT3	LP	1	1.0018e-02	3.1178e-05
CT3	LOS	1	5.5735e-03	9.4146e-06
CT3	LP2	1	8.0132e-03	2.9568e-05
CT3	LP3	1	9.7944e-03	3.6141e-05
CT3	LC3	1	1.0113e-02	3.7316e-05
CT3	LC2	1	8.0668e-03	2.6311e-05
CLA	LO	1	4.2060e-03	5.9555e-06
CLA	LOM	1	4.2060e-03	5.9555e-06
CLA	LNL	1	4.8796e-03	8.9087e-06
CLA	LC	1	5.8048e-03	1.6040e-05
CLA	LH1	1	5.2711e-03	1.5158e-05
CLA	LH2	1	6.9559e-03	2.1733e-05
CLA	LP	1	7.9453e-03	2.1779e-05
CLA	LOS	1	4.3599e-03	6.3977e-06
CLA	LP2	1	6.3781e-03	2.0803e-05
CLA	LP3	1	7.7958e-03	2.5427e-05
CLA	LC3	1	8.0493e-03	2.6254e-05
CLA	LC2	1	6.4041e-03	1.8416e-05
CF3	LO	1	8.0775e-03	2.1268e-05
CF3	LOM	1	8.0775e-03	2.1268e-05
CF3	LNL	1	9.1445e-03	3.0294e-05
CF3	LC	1	1.0473e-02	5.0554e-05
CF3	LH1	1	9.4765e-03	4.7439e-05

CF3	LH2	1	1.2415e-02	6.7034e-05
CF3	LP	1	1.4345e-02	6.8741e-05
CF3	LOS	1	8.3438e-03	2.2688e-05
CF3	LP2	1	1.1341e-02	6.3688e-05
CF3	LP3	1	1.3862e-02	7.7845e-05
CF3	LC3	1	1.4313e-02	8.0376e-05
CF3	LC2	1	1.1513e-02	5.7635e-05
NF	LO	1	2.8338e-03	2.5395e-06
NF	LOM	1	2.8338e-03	2.5395e-06
NF	LNL	1	3.3531e-03	3.9513e-06
NF	LC	1	4.1113e-03	7.5576e-06
NF	LH1	1	3.7437e-03	7.1822e-06
NF	LH2	1	4.9688e-03	1.0417e-05
NF	LP	1	5.6241e-03	1.0250e-05
NF	LOS	1	2.9458e-03	2.7435e-06
NF	LP2	1	4.5695e-03	1.0030e-05
NF	LP3	1	5.5852e-03	1.2259e-05
NF	LC3	1	5.7668e-03	1.2658e-05
NF	LC2	1	4.5484e-03	8.7260e-06
SF	LO	1	4.6201e-03	5.5661e-06
SF	LOM	1	4.6201e-03	5.5661e-06
SF	LNL	1	5.3965e-03	8.4401e-06
SF	LC	1	6.4872e-03	1.5517e-05
SF	LH1	1	5.8965e-03	1.4692e-05
SF	LH2	1	7.7967e-03	2.1150e-05
SF	LP	1	8.8776e-03	2.1061e-05
SF	LOS	1	4.7938e-03	5.9911e-06
SF	LP2	1	7.1563e-03	2.0286e-05
SF	LP3	1	8.7469e-03	2.4795e-05
SF	LC3	1	9.0314e-03	2.5602e-05
SF	LC2	1	7.1639e-03	1.7851e-05
OF	LO	1	2.3639e-03	1.5899e-06
OF	LOM	1	2.3639e-03	1.5899e-06
OF	LNL	1	2.8339e-03	2.5395e-06
OF	LC	1	3.5448e-03	5.0553e-06
OF	LH1	1	3.2338e-03	4.8219e-06
OF	LH2	1	4.3083e-03	7.0464e-06
OF	LP	1	4.8474e-03	6.8514e-06
OF	LOS	1	2.4619e-03	1.7241e-06
OF	LP2	1	3.9697e-03	6.8111e-06
OF	LP3	1	4.8521e-03	8.3250e-06
OF	LC3	1	5.0099e-03	8.5958e-06
OF	LC2	1	3.9289e-03	5.8584e-06
PP	LO	1	4.8480e-03	6.8522e-06
PP	LOM	1	4.8480e-03	6.8522e-06
PP	LNL	1	5.6248e-03	1.0252e-05
PP	LC	1	6.6921e-03	1.8462e-05
PP	LH1	1	6.0769e-03	1.7447e-05
PP	LH2	1	8.0194e-03	2.5017e-05
PP	LP	1	9.1598e-03	2.5068e-05
PP	LOS	1	5.0254e-03	7.3612e-06
PP	LP2	1	7.3533e-03	2.3947e-05

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    PP   LP3     1  8.9878e-03  2.9270e-05
    PP   LC3     1  9.2801e-03  3.0221e-05
    PP   LC2     1  7.3831e-03  2.1198e-05
    FF    LO     1  1.5044e-03  1.1851e-06
    FF   LOM     1  1.5044e-03  1.1851e-06
    FF   LNL     1  1.7904e-03  1.8655e-06
    FF    LC     1  2.2148e-03  3.6319e-06
    FF   LH1     1  2.0185e-03  3.4572e-06
    FF   LH2     1  2.6835e-03  5.0310e-06
    FF    LP     1  3.0293e-03  4.9243e-06
    FF   LOS     1  1.5651e-03  1.2824e-06
    FF   LP2     1  2.4699e-03  4.8525e-06
    FF   LP3     1  3.0189e-03  5.9311e-06
    FF   LC3     1  3.1171e-03  6.1240e-06
    FF   LC2     1  2.4523e-03  4.2003e-06
    BB    LO     1  2.9053e-03  3.5521e-06
    BB   LOM     1  2.9053e-03  3.5521e-06
    BB   LNL     1  3.3915e-03  5.3794e-06
    BB    LC     1  4.0730e-03  9.8709e-06
    BB   LH1     1  3.7018e-03  9.3448e-06
    BB   LH2     1  4.8938e-03  1.3447e-05
    BB    LP     1  5.5739e-03  1.3398e-05
    BB   LOS     1  3.0143e-03  3.8226e-06
    BB   LP2     1  4.4915e-03  1.2895e-05
    BB   LP3     1  5.4898e-03  1.5762e-05
    BB   LC3     1  5.6683e-03  1.6274e-05
    BB   LC2     1  4.4975e-03  1.1353e-05
;;IL-water nonbond interactions
    NA    OW     1  2.9649e-03  3.2316e-06
    NA     H     1  0.0000e+00  0.0000e+00
    CR    OW     1  2.4224e-03  3.0330e-06
    CR     H     1  0.0000e+00  0.0000e+00
    CW    OW     1  2.4224e-03  3.0330e-06
    CW     H     1  0.0000e+00  0.0000e+00
    H5    OW     1  1.3188e-04  1.5219e-08
    H5     H     1  0.0000e+00  0.0000e+00
    H4    OW     1  2.1031e-04  3.8708e-08
    H4     H     1  0.0000e+00  0.0000e+00
   CN3    OW     1  5.1920e-03  9.3738e-06
   CN3     H     1  0.0000e+00  0.0000e+00
   CN2    OW     1  4.5234e-03  8.2300e-06
   CN2     H     1  0.0000e+00  0.0000e+00
   CTA    OW     1  4.8690e-03  9.8532e-06
   CTA     H     1  0.0000e+00  0.0000e+00
   CT2    OW     1  4.8690e-03  9.8532e-06
   CT2     H     1  0.0000e+00  0.0000e+00
   CT3    OW     1  5.5280e-03  1.0769e-05
   CT3     H     1  0.0000e+00  0.0000e+00
   CLA    OW     1  4.3387e-03  7.3670e-06
   CLA     H     1  0.0000e+00  0.0000e+00
   CF3    OW     1  8.1870e-03  2.5399e-05
   CF3     H     1  0.0000e+00  0.0000e+00
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    NF    OW     1  2.9649e-03  3.2316e-06
    NF     H     1  0.0000e+00  0.0000e+00
    SF    OW     1  4.7892e-03  6.9530e-06
    SF     H     1  0.0000e+00  0.0000e+00
    OF    OW     1  2.4967e-03  2.0618e-06
    OF     H     1  0.0000e+00  0.0000e+00
    PP    OW     1  5.0012e-03  8.4772e-06
    PP     H     1  0.0000e+00  0.0000e+00
    FF    OW     1  1.5806e-03  1.5207e-06
    FF     H     1  0.0000e+00  0.0000e+00
    BB    OW     1  3.0103e-03  4.4331e-06
    BB     H     1  0.0000e+00  0.0000e+00

[ pairtypes ]
; IL 1-4 interactions
    NA    NA     1  1.6764e-03  1.9755e-06
    NA    CR     1  1.3672e-03  1.8475e-06
    NA    CW     1  1.3672e-03  1.8475e-06
    NA    H5     1  7.7226e-05  9.9798e-09
    NA    H4     1  1.2213e-04  2.4960e-08
    NA   CN3     1  2.9173e-03  5.6589e-06
    NA   CN2     1  2.5413e-03  4.9675e-06
    NA   CTA     1  2.7321e-03  5.9324e-06
    NA   CT2     1  2.7321e-03  5.9324e-06
    NA   CT3     1  3.1033e-03  6.4894e-06
    NA   CLA     1  2.4396e-03  4.4540e-06
    NA   CF3     1  4.5718e-03  1.5146e-05
    NA    NF     1  1.6764e-03  1.9755e-06
    NA    SF     1  2.6980e-03  4.2197e-06
    NA    OF     1  1.4168e-03  1.2697e-06
    CR    CR     1  1.1117e-03  1.7174e-06
    CR    CW     1  1.1117e-03  1.7174e-06
    CR    H5     1  6.6879e-05  1.0523e-08
    CR    H4     1  1.0427e-04  2.5579e-08
    CR   CN3     1  2.3538e-03  5.1794e-06
    CR   CN2     1  2.0501e-03  4.5451e-06
    CR   CTA     1  2.1993e-03  5.4045e-06
    CR   CT2     1  2.1993e-03  5.4045e-06
    CR   CT3     1  2.4999e-03  5.9211e-06
    CR   CLA     1  1.9709e-03  4.0869e-06
    CR   CF3     1  3.6496e-03  1.3570e-05
    CR    NF     1  1.3673e-03  1.8476e-06
    CR    SF     1  2.1868e-03  3.8975e-06
    CR    OF     1  1.1629e-03  1.2025e-06
    CW    CW     1  1.1117e-03  1.7174e-06
    CW    H5     1  6.6879e-05  1.0523e-08
    CW    H4     1  1.0427e-04  2.5579e-08
    CW   CN3     1  2.3538e-03  5.1794e-06
    CW   CN2     1  2.0501e-03  4.5451e-06
    CW   CTA     1  2.1993e-03  5.4045e-06
    CW   CT2     1  2.1993e-03  5.4045e-06
    CW   CT3     1  2.4999e-03  5.9211e-06
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CW	CLA	1	1.9709e-03	4.0869e-06
CW	CF3	1	3.6496e-03	1.3570e-05
CW	NF	1	1.3673e-03	1.8476e-06
CW	SF	1	2.1868e-03	3.8975e-06
CW	OF	1	1.1629e-03	1.2025e-06
H5	H5	1	9.4393e-07	3.5493e-12
H5	H4	1	2.1064e-06	1.7675e-11
H5	CN3	1	1.6568e-04	4.3452e-08
H5	CN2	1	1.4477e-04	3.8374e-08
H5	CTA	1	1.6216e-04	4.9748e-08
H5	CT2	1	1.6216e-04	4.9748e-08
H5	CT3	1	1.8152e-04	5.2855e-08
H5	CLA	1	1.3525e-04	3.2586e-08
H5	CF3	1	3.1693e-04	1.7326e-07
H5	NF	1	7.7227e-05	9.9799e-09
H5	SF	1	1.4041e-04	2.7203e-08
H5	OF	1	5.7536e-05	4.9842e-09
H4	H4	1	4.2753e-06	7.2811e-11
H4	CN3	1	2.4942e-04	9.8470e-08
H4	CN2	1	2.1778e-04	8.6841e-08
H4	CTA	1	2.4163e-04	1.1046e-07
H4	CT2	1	2.4163e-04	1.1046e-07
H4	CT3	1	2.7140e-04	1.1815e-07
H4	CLA	1	2.0475e-04	7.4682e-08
H4	CF3	1	4.5578e-04	3.5833e-07
H4	NF	1	1.2213e-04	2.4960e-08
H4	SF	1	2.1573e-04	6.4219e-08
H4	OF	1	9.3794e-05	1.3246e-08
CN3	CN3	1	4.8863e-03	1.5017e-05
CN3	CN2	1	4.2542e-03	1.3167e-05
CN3	CTA	1	4.5385e-03	1.5485e-05
CN3	CT2	1	4.5385e-03	1.5485e-05
CN3	CT3	1	5.1692e-03	1.7032e-05
CN3	CLA	1	4.1046e-03	1.1926e-05
CN3	CF3	1	7.3726e-03	3.7256e-05
CN3	NF	1	2.9173e-03	5.6590e-06
CN3	SF	1	4.5927e-03	1.1566e-05
CN3	OF	1	2.5212e-03	3.8029e-06
CN2	CN2	1	3.7039e-03	1.1545e-05
CN2	CTA	1	3.9510e-03	1.3574e-05
CN2	CT2	1	3.9510e-03	1.3574e-05
CN2	CT3	1	4.5001e-03	1.4931e-05
CN2	CLA	1	3.5739e-03	1.0459e-05
CN2	CF3	1	6.4153e-03	3.2630e-05
CN2	NF	1	2.5414e-03	4.9676e-06
CN2	SF	1	3.9996e-03	1.0146e-05
CN2	OF	1	2.1970e-03	3.3404e-06
CTA	CTA	1	4.2080e-03	1.5910e-05
CTA	CT2	1	4.2080e-03	1.5910e-05
CTA	CT3	1	4.7956e-03	1.7520e-05
CTA	CLA	1	3.8162e-03	1.2322e-05
CTA	CF3	1	6.7917e-03	3.7789e-05

```
   CTA    NF     1  2.7322e-03  5.9325e-06
   CTA    SF     1  4.2808e-03  1.2010e-05
   CTA    OF     1  2.3725e-03  4.0250e-06
   CT2   CT2     1  4.2080e-03  1.5910e-05
   CT2   CT3     1  4.7956e-03  1.7520e-05
   CT2   CLA     1  3.8162e-03  1.2322e-05
   CT2   CF3     1  6.7917e-03  3.7789e-05
   CT2    NF     1  2.7322e-03  5.9325e-06
   CT2    SF     1  4.2808e-03  1.2010e-05
   CT2    OF     1  2.3725e-03  4.0250e-06
   CT3   CT3     1  5.4641e-03  1.9286e-05
   CT3   CLA     1  4.3451e-03  1.3544e-05
   CT3   CF3     1  7.7566e-03  4.1792e-05
   CT3    NF     1  3.1033e-03  6.4895e-06
   CT3    SF     1  4.8700e-03  1.3179e-05
   CT3    OF     1  2.6905e-03  4.3889e-06
   CLA   CLA     1  3.4462e-03  9.4615e-06
   CLA   CF3     1  6.2210e-03  2.9855e-05
   CLA    NF     1  2.4396e-03  4.4540e-06
   CLA    SF     1  3.8507e-03  9.1503e-06
   CLA    OF     1  2.1029e-03  2.9776e-06
   CF3   CF3     1  1.0708e-02  8.5652e-05
   CF3    NF     1  4.5719e-03  1.5146e-05
   CF3    SF     1  7.0420e-03  2.9632e-05
   CF3    OF     1  4.0385e-03  1.0634e-05
    NF    NF     1  1.6764e-03  1.9755e-06
    NF    SF     1  2.6981e-03  4.2198e-06
    NF    OF     1  1.4168e-03  1.2697e-06
    SF    SF     1  4.2873e-03  8.7865e-06
    SF    OF     1  2.3099e-03  2.7829e-06
    OF    OF     1  1.1819e-03  7.9492e-07
; Lipid 1-4 interactions, note that these interactions are half of what's given in
;the orignal lipid force field because the pairs are listed twice in the lipid itp
;to account for the fact that the electrostatic scaling is 0.5 for the IL and 1.0
;for lipids
LO      LO      1       1.47600E-04     9.93500E-08
LO      LOM     1       1.47600E-04     9.93500E-08
LO      OW      1       1.56400E-04     1.29200E-07
LO      LNL     1       1.75900E-04     1.56650E-07
LO      LC      1       2.12300E-04     2.90450E-07
LO      LH1     1       1.92750E-04     2.74500E-07
LO      LH2     1       2.54100E-04     3.92600E-07
LO      H       1       0.00000E+00     0.00000E+00
LO      LP      1       2.90650E-04     3.94500E-07
LO      LOS     1       1.53750E-04     1.07650E-07
LO      LP2     1       2.32850E-04     3.75000E-07
LO      LP3     1       2.84500E-04     4.58400E-07
LO      LC3     1       2.93800E-04     4.73300E-07
LO      LC2     1       2.34250E-04     3.33400E-07
LOM     LOM     1       1.47600E-04     9.93500E-08
LOM     OW      1       1.56400E-04     1.29200E-07
LOM     LNL     1       1.75900E-04     1.56650E-07
```

LOM	LC	1	2.12300E-04	2.90450E-07
LOM	LH1	1	1.92750E-04	2.74500E-07
LOM	LH2	1	2.54100E-04	3.92600E-07
LOM	H	1	0.00000E+00	0.00000E+00
LOM	LP	1	2.90650E-04	3.94500E-07
LOM	LOS	1	1.53750E-04	1.07650E-07
LOM	LP2	1	2.32850E-04	3.75000E-07
LOM	LP3	1	2.84500E-04	4.58400E-07
LOM	LC3	1	2.93800E-04	4.73300E-07
LOM	LC2	1	2.34250E-04	3.33400E-07
OW	LNL	1	1.86350E-04	2.03700E-07
OW	LC	1	2.24900E-04	3.77800E-07
OW	LH1	1	2.04250E-04	3.57050E-07
OW	LH2	1	2.69250E-04	5.10500E-07
OW	H	1	0.00000E+00	0.00000E+00
OW	LP	1	3.07950E-04	5.13000E-07
OW	LOS	1	1.62900E-04	1.40050E-07
OW	LP2	1	2.46700E-04	4.87700E-07
OW	LP3	1	3.01450E-04	5.96000E-07
OW	LC3	1	3.11300E-04	6.15500E-07
OW	LC2	1	2.48200E-04	4.33650E-07
LNL	LNL	1	2.09600E-04	2.47000E-07
LNL	LC	1	2.52950E-04	4.58050E-07
LNL	LH1	1	2.29700E-04	4.32850E-07
LNL	LH2	1	3.02800E-04	6.19000E-07
LNL	H	1	0.00000E+00	0.00000E+00
LNL	LP	1	3.46350E-04	6.22000E-07
LNL	LOS	1	1.83250E-04	1.69800E-07
LNL	LP2	1	2.77450E-04	5.91500E-07
LNL	LP3	1	3.39050E-04	7.23000E-07
LNL	LC3	1	3.50150E-04	7.46500E-07
LNL	LC2	1	2.79150E-04	5.25500E-07
LC	LC	1	3.05300E-04	8.49500E-07
LC	LH1	1	2.77250E-04	8.02500E-07
LC	LH2	1	3.65400E-04	1.14800E-06
LC	H	1	0.00000E+00	0.00000E+00
LC	LP	1	4.18000E-04	1.15350E-06
LC	LOS	1	2.21100E-04	3.14850E-07
LC	LP2	1	3.34850E-04	1.09650E-06
LC	LP3	1	4.09150E-04	1.34050E-06
LC	LC3	1	4.22550E-04	1.38400E-06
LC	LC2	1	3.36850E-04	9.75000E-07
LH1	LH1	1	2.51750E-04	7.58500E-07
LH1	LH2	1	3.31850E-04	1.08500E-06
LH1	H	1	0.00000E+00	0.00000E+00
LH1	LP	1	3.79600E-04	1.09000E-06
LH1	LOS	1	2.00800E-04	2.97550E-07
LH1	LP2	1	3.04100E-04	1.03650E-06
LH1	LP3	1	3.71550E-04	1.26700E-06
LH1	LC3	1	3.83700E-04	1.30800E-06
LH1	LC2	1	3.05900E-04	9.21500E-07
LH2	LH2	1	4.37400E-04	1.55200E-06

LH2	H	1	0.00000E+00	0.00000E+00
LH2	LP	1	5.00500E-04	1.55950E-06
LH2	LOS	1	2.64700E-04	4.25600E-07
LH2	LP2	1	4.00800E-04	1.48200E-06
LH2	LP3	1	4.89750E-04	1.81200E-06
LH2	LC3	1	5.06000E-04	1.87100E-06
LH2	LC2	1	4.03250E-04	1.31800E-06
H	H	1	0.00000E+00	0.00000E+00
H	LP	1	0.00000E+00	0.00000E+00
H	LOS	1	0.00000E+00	0.00000E+00
H	LP2	1	0.00000E+00	0.00000E+00
H	LP3	1	0.00000E+00	0.00000E+00
H	LC3	1	0.00000E+00	0.00000E+00
H	LC2	1	0.00000E+00	0.00000E+00
LP	LP	1	5.72500E-04	1.56650E-06
LP	LOS	1	3.02750E-04	4.27600E-07
LP	LP2	1	4.58450E-04	1.48900E-06
LP	LP3	1	5.60000E-04	1.82050E-06
LP	LC3	1	5.78500E-04	1.88000E-06
LP	LC2	1	4.61250E-04	1.32400E-06
LOS	LOS	1	1.60150E-04	1.16700E-07
LOS	LP2	1	2.42550E-04	4.06450E-07
LOS	LP3	1	2.96350E-04	4.96900E-07
LOS	LC3	1	3.06050E-04	5.13000E-07
LOS	LC2	1	2.44000E-04	3.61400E-07
LP2	LP2	1	3.67300E-04	1.41550E-06
LP2	LP3	1	4.48750E-04	1.73050E-06
LP2	LC3	1	4.63450E-04	1.78700E-06
LP2	LC2	1	3.69500E-04	1.25850E-06
LP3	LP3	1	5.48500E-04	2.11550E-06
LP3	LC3	1	5.66500E-04	2.18450E-06
LP3	LC2	1	4.51500E-04	1.53850E-06
LC3	LC3	1	5.85000E-04	2.25550E-06
LC3	LC2	1	4.66250E-04	1.58850E-06
LC2	LC2	1	3.71750E-04	1.11900E-06

MD Parameters

example_npt.mdp

```
integrator        = md
dt                = 0.002
nsteps                = 5000000

; Parameters controlling output writing
nstxout                = 5000
nstvout                = 5000
nstenergy        = 5000
nstlog                = 5000

ns_type                = grid
nstlist                = 5
rlist                = 1.2
rcoulomb        = 1.2
rvdw                = 1.2
pbc                = xyz

; Parameters for treating bonded interactions
continuation        = yes
constraint_algorithm = LINCS
constraints        = all-bonds
lincs_iter        = 1
lincs_order        = 4

coulombtype        = PME
pme_order        = 4

; Temperature coupling parameters
tcoupl                = Nose-Hoover
tc-grps                = POP        BMI_CLA_SOL
tau_t                = 0.5        0.5
ref_t                = 298        298

; Pressure coupling parameters
pcoupl                = Parrinello-Rahman
pcoupltype        = semiisotropic
tau_p                = 5.0
ref_p                = 1.0        1.0
compressibility = 4.5e-5        4.5e-5
DispCorr        = no
gen_vel                = no
nstcomm                = 1
comm_mode        = Linear
comm_grps        = POP BMI CLA SOL
```

example_pull.mdp

```
title       = pulling simulation

integrator  = md
dt          = 0.002
tinit       = 0
nsteps      = 250000
nstcomm     = 10

nstxout     = 5000
nstvout     = 5000
nstfout     = 500
nstxtcout   = 500
nstenergy   = 500

constraint_algorithm    = lincs
constraints             = all-bonds
continuation            = no

nstlist     = 5
ns_type     = grid
rlist       = 1.2
rcoulomb    = 1.2
rvdw        = 1.2

coulombtype     = PME
fourierspacing  = 0.16
fourier_nx      = 0
fourier_ny      = 0
fourier_nz      = 0
pme_order       = 4
ewald_rtol      = 1e-5
optimize_fft    = yes

Tcoupl      = Nose-Hoover
tc_grps     = POP   BMI_CLA_SOL
tau_t       = 0.5       0.5
ref_t       = 298       298

Pcoupl          = Parrinello-Rahman
pcoupltype      = semiisotropic
tau_p           = 5.0
compressibility = 4.5e-5 4.5e-5
ref_p           = 1.0 1.0
refcoord_scaling = com
gen_vel     = no
pbc     = xyz
DispCorr    = no

pull            = umbrella
pull_geometry   = distance
```

```
pull_dim        = N N Y
pull_start      = yes
pull_ngroups    = 1
pull_group0     = POP
pull_group1     = CLA
pull_rate1      = -0.01
pull_k1         = 1000
comm_mode       = Linear
comm_grps       = POP BMI CLA SOL
```

example_umbrella.mdp

```
title       = Umbrella simulation

integrator  = md
dt          = 0.002
tinit       = 0
nsteps      = 5000000
nstcomm     = 1

nstxout     = 5000
nstvout     = 5000
nstfout     = 5000
nstxtcout   = 5000
nstenergy   = 5000

constraint_algorithm    = lincs
constraints             = all-bonds
continuation            = yes
nstlist     = 5
ns_type     = grid
rlist       = 1.2
rcoulomb    = 1.2
rvdw        = 1.2
coulombtype     = PME
fourierspacing  = 0.16
fourier_nx      = 0
fourier_ny      = 0
fourier_nz      = 0
pme_order       = 4
ewald_rtol      = 1e-5
optimize_fft    = yes

Tcoupl      = Nose-Hoover
tc_grps     = POP   BMI_CLA_SOL
tau_t       = 0.5       0.5
ref_t       = 298       298

Pcoupl          = Parrinello-Rahman
pcoupltype      = semiisotropic
tau_p           = 5.0 5.0
```

```
compressibility = 4.5e-5 4.5e-5
ref_p           = 1.0 1.0

refcoord_scaling = com
gen_vel     = no
pbc     = xyz
DispCorr    = no

pull            = umbrella
pull_geometry   = distance
pull_dim        = N N Y
pull_start      = yes
pull_ngroups    = 1
pull_group0     = POP
pull_group1     = CLA
pull_init1      = 0
pull_rate1      = 0.0
pull_k1         = 1000
pull_nstxout    = 100
pull_nstfout    = 100
comm_mode       = Linear
comm_grps       = POP BMI CLA SOL
```