Complementary Molecular Dynamics and X-ray Reflectivity Study of Ionic Liquids at Solid Interfaces

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Computational Details. A fully hydroxylated (0001) surface of sapphire, representing the most stable termination facet of natural sapphire crystal, was parametrized using the CLAYFF force field.[1] The surface was prepared in Material Studio[2] following optimization of the unit cell parameters performed in GULP,[3] thereby producing an 82.4 Å x 62.9 Å x 21.2 Å box, for which the *z*-axis corresponds to the surface normal. The model IL ([C_2Mim][NTf_2], schematic representation and atom labeling shown in Figure S1) was parametrized using two specialized IL force fields, namely the Ludwig et al.[4] and Maginn[5]/Canongia Lopes et al.[6] force fields. To couple sapphire with the two different [C_2Mim][NTf_2] force fields, we employed both the geometric and Lorentz-Berthelot mixing rules in order to obtain the missing IL–sapphire Lennard–Jones potentials, thereby obtaining four distinct parametrizations of the system. These are namely, LG, LL, MG, and ML, where L and M correspond to the Ludwig–CLAYFF and Maginn/Canongia Lopes–CLAYFF combined force fields respectively, while G and L correspond to geometric and Lorentz–Berthelot mixing rules, respectively. The MD simulations, which were all performed with a timestep of 2 fs using GROMACS 4.5.5,[7] were carried out as follows:

(a) The pure ionic liquid, consisting of 1686 pairs of [C_2Mim][NTf_2] (box size 82.4 Å x 62.9 Å x 140.0 Å), was first minimized and then equilibrated for 0.6 ns at 600 K, which was followed by simulated annealing for 2 ns starting at 600 K and finishing at 300 K.

(b) The obtained IL box was combined with the sapphire surface such that the box size of combined system ≈ 82.4 Å x 62.9 Å x 164.2 Å, while the smallest distance of the ionic liquid to the sapphire surface was set to approximately 3 Å. Four semi-isotropic NPT simulations (P = 1 atm, $\beta = 4.8\times10^{-5}$ MPa^{-1}) corresponding to four parametrizations of the combined system were each performed for 1.4 ns, where box size in the *x* and *y* direction was held fixed, thereby enabling only *z* component to change. The average value of the *z* component over the final 1 ns (convergence seen after 0.3 ns) was used in the subsequent NVT simulations, respectively for all four parametrizations.

(c) The four model systems were then subjected to simulated annealing, starting at 600 K and finishing at 300 K (12 ns), with the number of particles and box size maintained constant.

(d) The obtained model systems were further simulated under NVT conditions, at T = 300 K, for 100 ns, constituting production runs (simulation box obtained from the production run of ML is shown in Figure S2).

Three-dimensional periodic boundary conditions were enforced in all aforementioned simulations. Both van der Waals and short range Coulomb interactions were cut at 12 Å, while long-range electrostatics was accounted for by employing the particle mesh Ewald procedure. The box length in the *z* direction (≈161 Å for all four cases) is enough to ensure that the mid-section (60–80 Å from the surface) of the simulation box possesses bulk-like properties.

To generate reflectivity curves from the MD simulations, electron density profiles with a bin size of 0.1 Å were extracted from the production runs. These profiles were convoluted with a Gaussian function of a width σ = 1.6 Å to simulate interfacial roughness that is present in the experimental system. This step does not influence the actual shape of features seen in the resulting reflectivities but rather changes the general decay of R/R_F, matching it to the experimental curve (Figure S6). Since CLAYFF underestimate sapphire bulk density for approximately 5% and density contrast makes difference when it comes to reflectivity, the substrate contribution was replaced by an error function $\rho_s = \frac{1}{2\rho_a}[1 + \mathrm{erf}\left(-\frac{z}{\sqrt{2}\sigma_s}\right)]$, centered around the

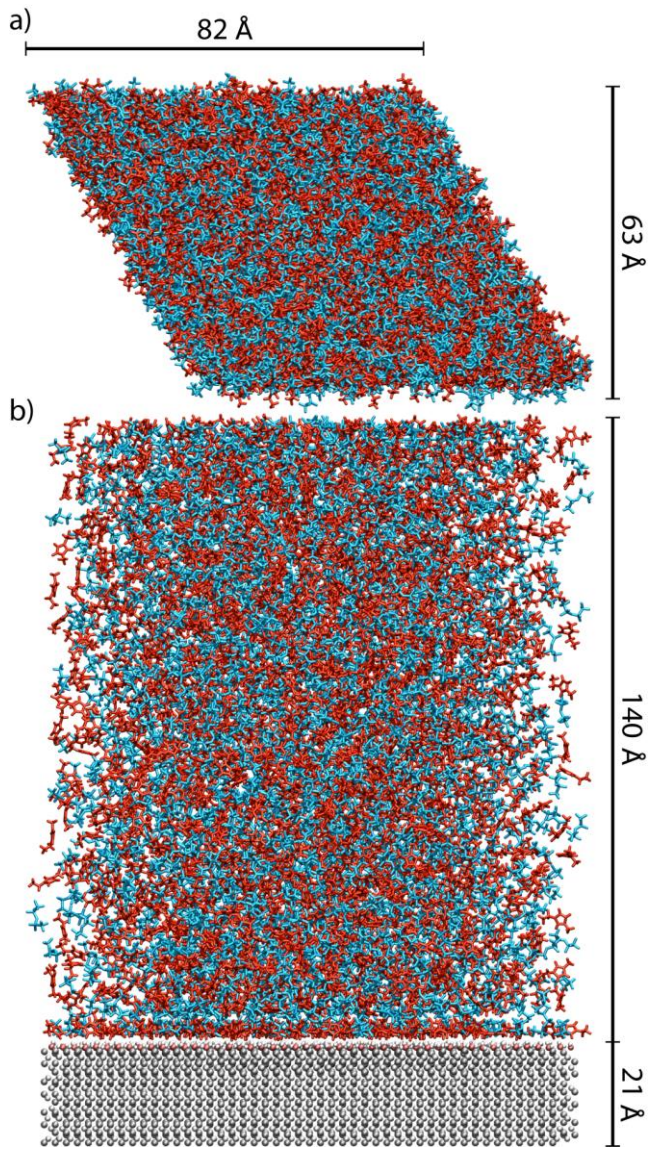
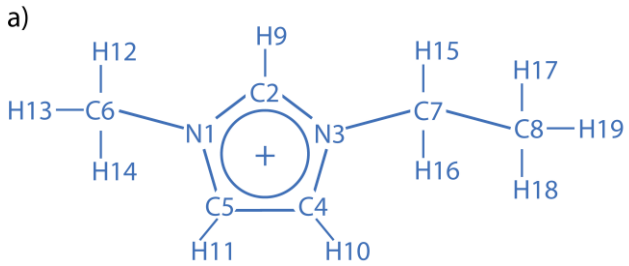


Figure S2. (a) Top and (b) side view of the monoclinic simulation box, with 1686 pairs of [C_2Mim][NTf_2] lying on 21 Å thick fully hydroxylated (0001) sapphire surface.



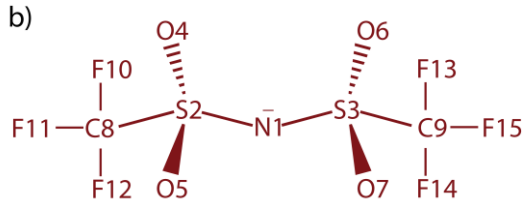


Figure S1. Schematic representation of (a) [C_2Mim]$^+$ and (b) [NTf_2]$^-$.

interface, where ρ_a= 1.184/Å^3 is the experimental bulk electron density of sapphire. On the liquid side, the profiles were cut off and continued with a constant liquid density value after a point where layering peaks become indistinguishable from bulk fluctuations that are inherent to the simulations. Cut-off points of 40 Å for LG and MG, and 60 Å for LL and ML systems were chosen on the basis of the unsmoothed number density profiles of cations and anions. Reflectivity curves are calculated from the resulting density profiles by applying the master formula.[8]

Experimental Section. Experimental X-ray reflectivity data was collected at the surface diffraction beamline 33-ID at the Advanced Photon Source, Argonne, National Laboratory, using a custom-built solid–liquid sample cell made out of PEEK to access the interface. The cell is 5 mm wide, and the X-ray beam (22.0 keV), focused to a vertical-by-horizontal size of 210x60 μm^2 at the spot of the sample, enters and exits the liquid phase through 0.5 mm strong sapphire windows.

Fresh samples of [C_2Mim][NTf_2] IL were synthesized for the experiment in analogy to the procedure described in Syntesis section of Supporting Information. Karl Fischer titration revealed a water content of about 1000 ppm at the time of the experiment. The sapphire substrates (53 mm x 5 mm x 0.5 mm, from CrysTec GMbH, Germany) were chemically cleaned using standard procedures (subsequent ultrasonic baths in ethanol, acetone and toluene for five minutes each) before being treated with piranha acid (equal parts of sulfuric (96%) and hydrogen-peroxide (30%)) for thirty minutes to remove organic adsorbants from the surface. The samples were subsequently rinsed with and then stored in purified water (18.2 MOhm) for several hours. Prior to the experiment, the substrates were dried on a heating plate at 70 °C and immediately wetted with IL once all traces of water were removed. The sample cell was then equipped with the freshly prepared sapphire and filled with liquid.

The reflectivity $R(q)$ of the system was recorded as a function of momentum transfer q. Using a Pilatus 100 K detector both specular signal and the underlying background, primarily caused by bulk liquid scattering when transmitting trough the sample cell, were measured in the same run.[9] To avoid beam damage, which has a visible influence of the reflectivity curve after an exposure of several seconds, the sample was translated perpendicular to the plane of incidence by 0.6 mm for every data point in the curve.

Synthesis of [C_2Mim][NTf_2]. The *bis*(trifluoromethane-sulfonyl)imide) (NTf_2) IL was prepared according to the following procedure: 0.5 mol of the relevant precursor (as ethylsulfate for [C_2Mim]$^+$) was mixed with 100 mL of acetonitrile (HPLC grade) and precipitated by adding diethyl ether (500 mL) (analytical grade). The viscous oily product was decanted and dried at 50 °C by means of a Rotavapor. The resulting very viscous oil was dissolved in deionized water (250 mL) and the solution decolorized with active charcoal. After careful filtration and cooling, solid Li[NTf_2] (1.1 eq. with respect to the starting material) was added to the solution, and the mixture was vigorously stirred for 60 min. After this time, methylene chloride (analytical grade) was added (100 mL) and the stirring was continued for further 30 min. Then, the whole mixture was transferred to a separatory funnel and allowed to settle. The lower organic phase was separated and washed with small volume of deionized water, until the washings tested negative to the $AgNO_3$ test for chloride. The methylene chloride solution was then transferred to a Rotavapor and dried at 80 °C/<5mbar for 16 h. The final product was obtained in > 85% yield as a low viscous liquid, whose identity was confirmed with NMR.

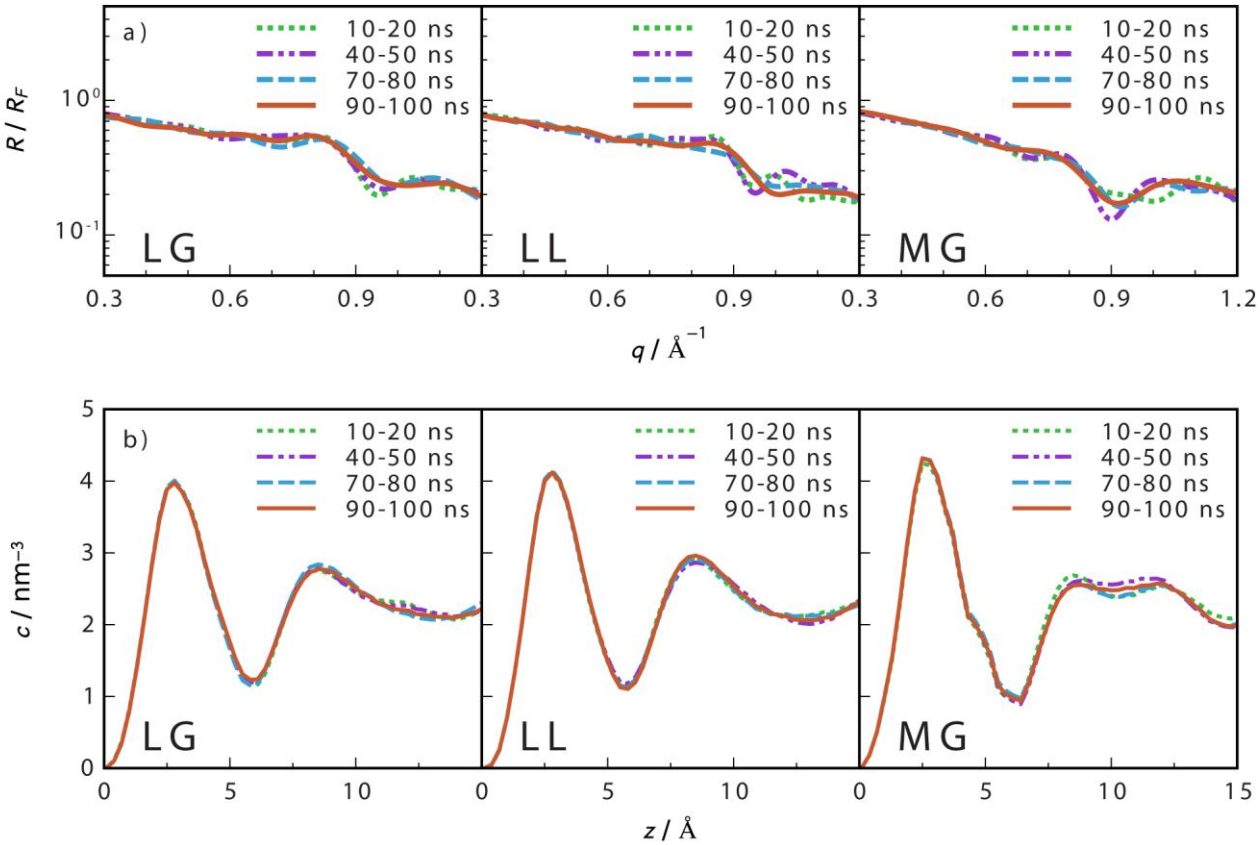


Figure S3. Time evolution of (a) reflectivities and (b) interface–normal number density profiles of cations, as obtained from MD simulations using LG, LL and MG parametrizations.

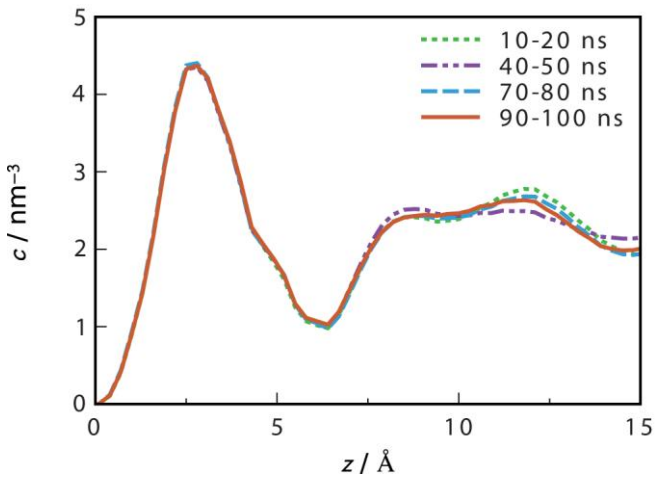


Figure S4. Time evolution of interface–normal number density profiles of cations, as obtained from MD simulations using ML parametrization.

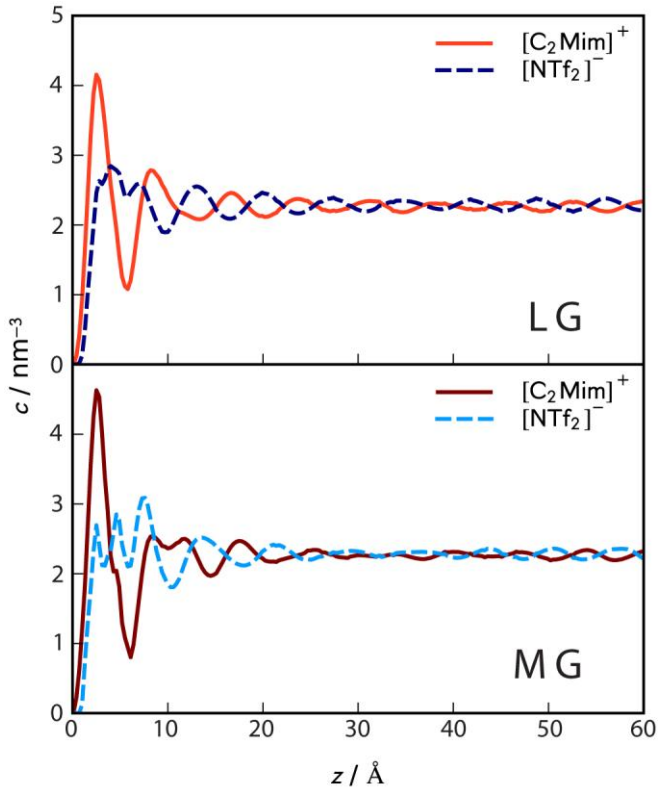


Figure S5. Interface–normal number density profiles of $[C_2Mim]^+$ and $[NTf_2]^-$ obtained from last 30 ns of a 100 ns long simulation, for LG and MG parametrizations of the IL–sapphire system.

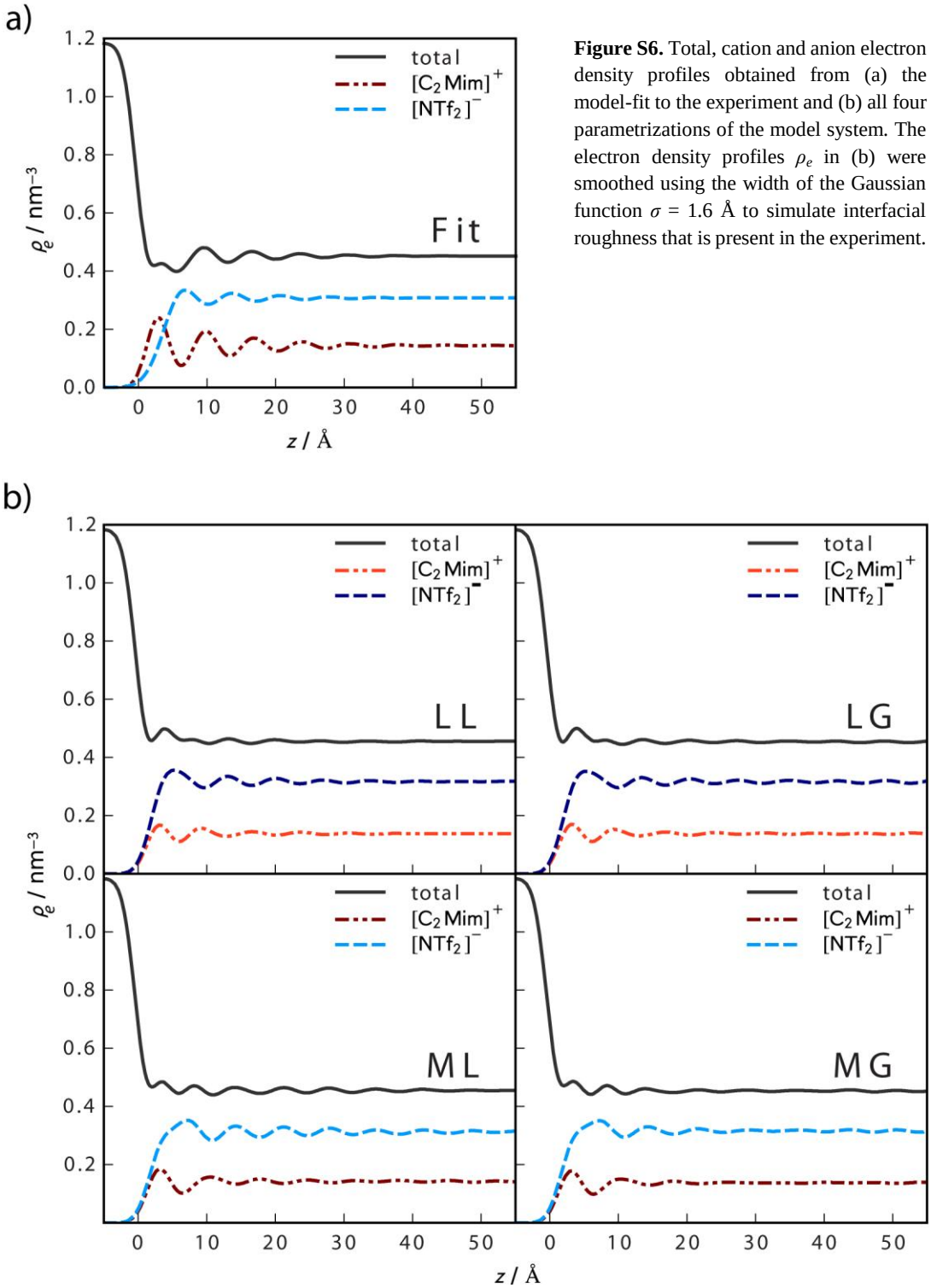


Figure S6. Total, cation and anion electron density profiles obtained from (a) the model-fit to the experiment and (b) all four parametrizations of the model system. The electron density profiles ρ_e in (b) were smoothed using the width of the Gaussian function σ = 1.6 Å to simulate interfacial roughness that is present in the experiment.

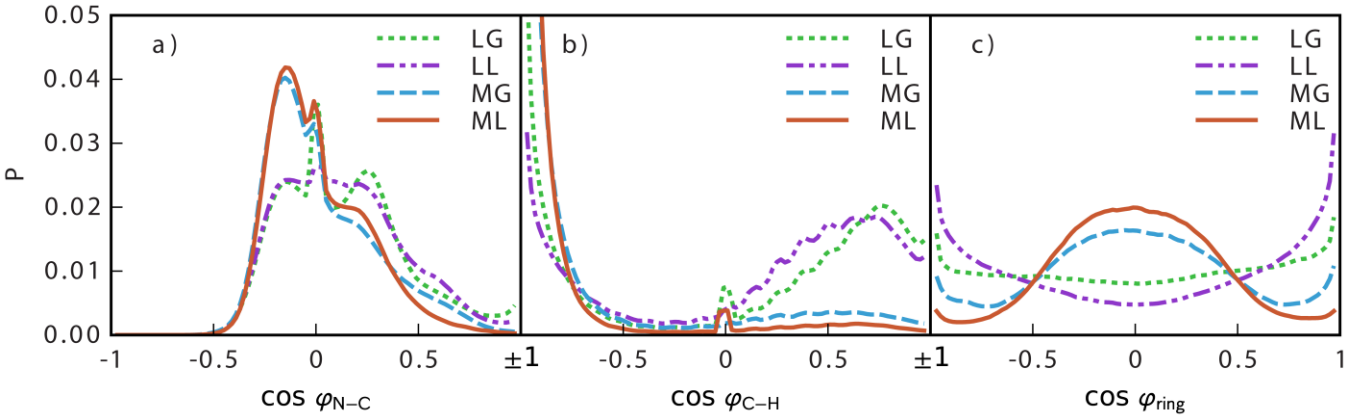


Figure S7. Probability distribution analysis of $[C_2Mim]^+$ in the first (interfacial) layer, for all four parametrizations. Non-normalized probability distribution is denoted with P, while $\varphi_{\mathbf{u}}$ represents the angle between the vector **u** and the unit vector **k (**normal to the surface). (a) N–C (N3–C8) vector, corresponding to the tail of the cation, (b) C–H (C2–H9) vector and (c) normal vector to the imidazolium ring, constructed as the cross product of the N1–C2 and N3–C2 vectors. Consult Figure S1 for the naming of the atoms.

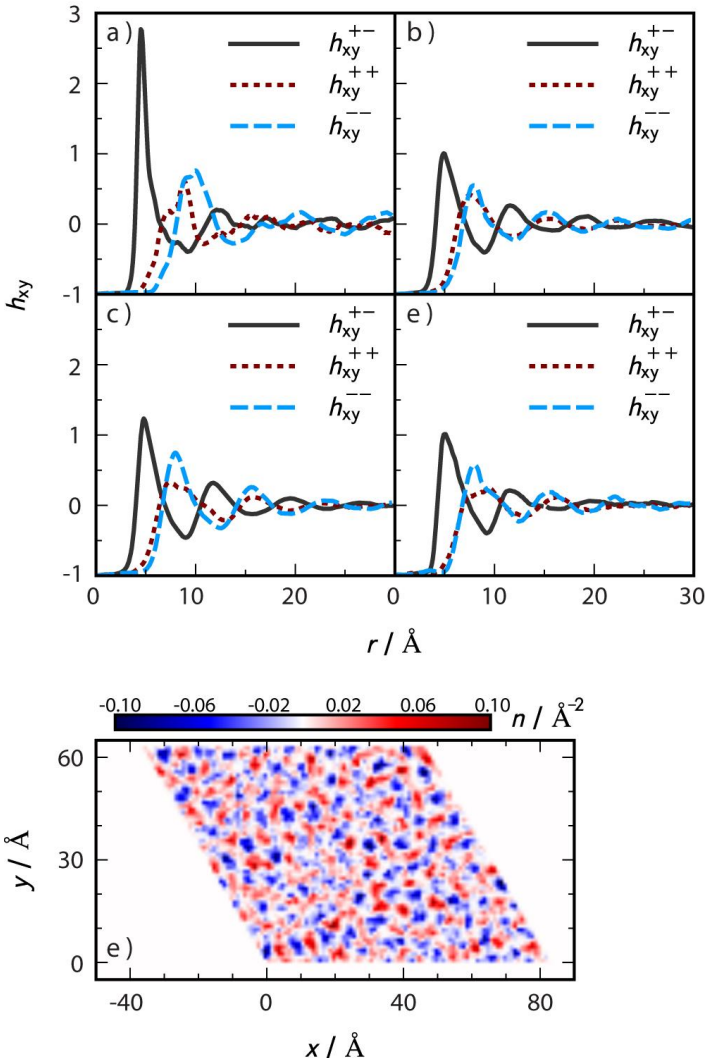


Figure S8. The anion–anion ($h_{xy}^{--}(r)$), cation–anion ($h_{xy}^{+-}(r)$) and the cation–cation ($h_{xy}^{++}(r)$) total in-plane correlation functions for (a) $4 < z < 6.5$ Å, (b) $23.5 < z < 26.7$ Å, (c) $26.7 < z < 30.4$ Å, and (d) $61 < z < 63$ Å (bulk). (e) 2D histogram of the in-plane positions of the ions in the bulk ($59 < z < 65$ Å). Correlation functions and the histograms are generated on the basis of the centers of mass of the constituent ions over the last 30 ns of the ML simulation.

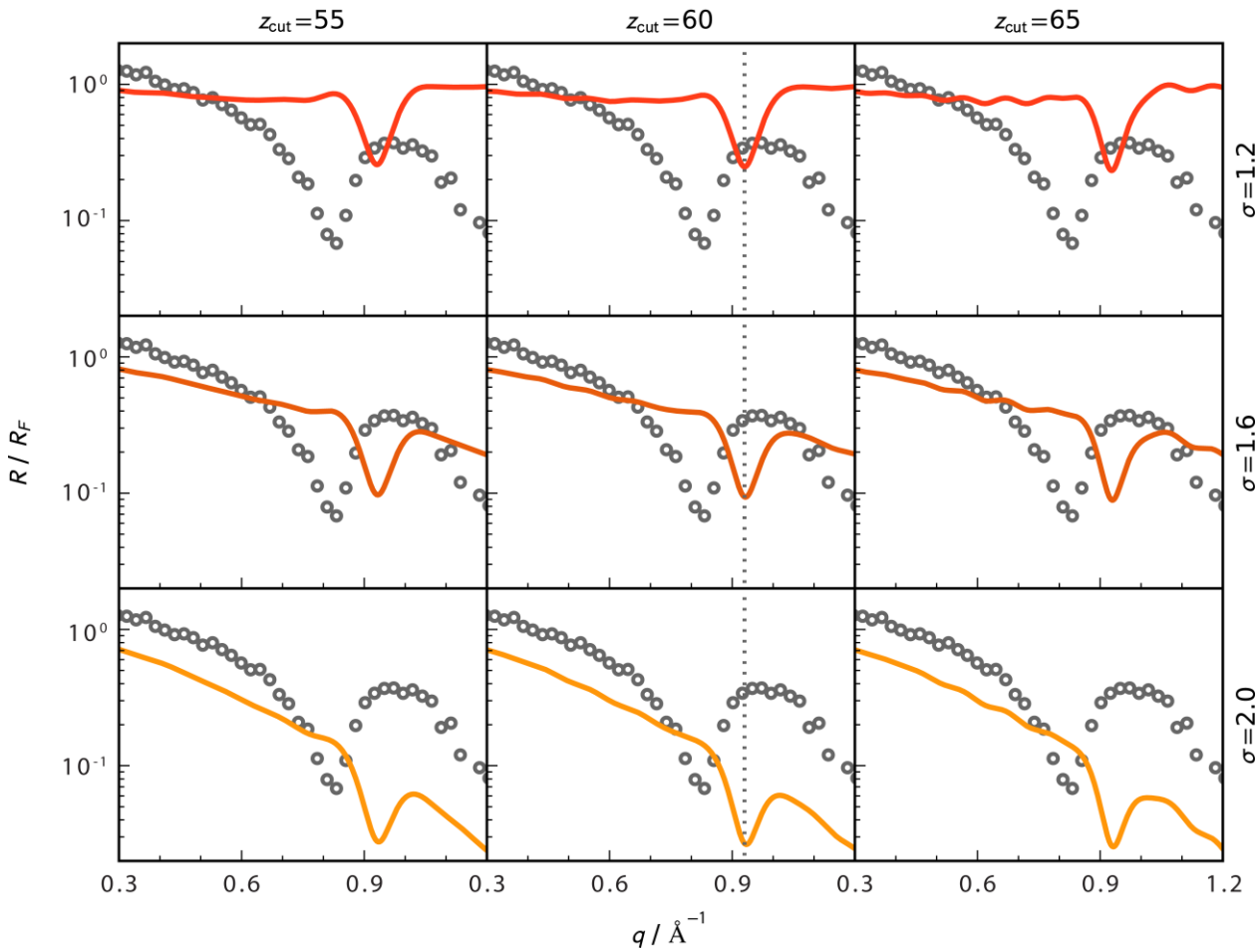


Figure S9. Reflectivity curves of ML obtained using different truncation distances (in Å, columns) and different smoothing, performed by convoluting with the Gaussian functions of width σ (in Å, rows), on the total electron density profile. The effect of smoothing is much more significant than the effect of the change in the truncation distance of ±5 Å around the chosen value (60 Å). However, the position of the predominant minimum in the reflectivity remains unaltered (2nd column).

Force Field Parameters. Atoms are labeled as in Figure S1.

Table S1. Assignment of the atoms for all four force fields.

$[C_2Mim]^+$ - labeling from Figure S1	Equivalent atom numbering for $[C_2Mim]^+$ in all four force fields (see [atoms] section of the force fields)	$[NTf_2]^-$ - labeling from Figure S1	Equivalent atom numbering for $[NTf_2]^-$ in all four force fields (see [atoms] section of the force fields)
N1	2	N1	8
C2	3	S2	4
N3	4	S3	9
C4	5	O4	5
C5	1	O5	7
C6	6	O6	10
C7	7	O7	11
C8	8	C8	1
H9	16	C9	12
H10	15	F10	2
H11	14	F11	3
H12	9	F12	6
H13	10	F13	13
H14	11	F14	14
H15	12	F15	15
H16	13		
H17	17		
H18	18		
H19	19		

Ludwig – Lorentz-Berthelot (LL)

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  11           h1           1            c2           h1           11           0.1300
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  2             6             9             1             0.110700E+03  0.313200E+03
  2             6             10            1             0.110700E+03  0.313200E+03
  2             6             11            1             0.110700E+03  0.313200E+03
  9             6             10            1             0.107800E+03  0.276200E+03
  9             6             11            1             0.107800E+03  0.276200E+03
  10            6             11            1             0.107800E+03  0.276200E+03
  4             7             8             1             0.112700E+03  0.418400E+03
  4             7             12            1             0.110700E+03  0.313200E+03
  4             7             13            1             0.110700E+03  0.313200E+03
  8             7             12            1             0.110700E+03  0.313200E+03
  8             7             13            1             0.110700E+03  0.313200E+03
  12            7             13            1             0.107800E+03  0.276200E+03
  7             8             17            1             0.110700E+03  0.313200E+03
  7             8             18            1             0.110700E+03  0.313200E+03
  7             8             19            1             0.110700E+03  0.313200E+03
  17            8             18            1             0.107800E+03  0.276200E+03
  17            8             19            1             0.107800E+03  0.276200E+03
  18            8             19            1             0.107800E+03  0.276200E+03

[ pairs ]
; i             j             func          sig           eps
  9             1             1             0.274660E+00  0.802092E-01
  9             3             1             0.230760E+00  0.117415E+00
  10            1             1             0.274660E+00  0.802092E-01
  10            3             1             0.230760E+00  0.117415E+00
  11            1             1             0.274660E+00  0.802092E-01
  11            3             1             0.230760E+00  0.117415E+00
  6             5             1             0.324980E+00  0.118969E+00
  6             14            1             0.268320E+00  0.778837E-01
  3             14            1             0.209320E+00  0.982359E-01
  2             15            1             0.258560E+00  0.124997E+00
  14            4             1             0.258560E+00  0.124997E+00
  14            15            1             0.205700E+00  0.439330E-01
  1             7             1             0.324980E+00  0.118969E+00
  15            3             1             0.209320E+00  0.982359E-01
  15            7             1             0.268320E+00  0.778837E-01
  5             16            1             0.209320E+00  0.982359E-01
  7             2             1             0.337270E+00  0.221593E+00
  7             16            1             0.225430E+00  0.114010E+00
  4             6             1             0.337270E+00  0.221593E+00
  16            6             1             0.225430E+00  0.114010E+00
  16            1             1             0.209320E+00  0.982359E-01
  5             12            1             0.274660E+00  0.802092E-01
  5             13            1             0.274660E+00  0.802092E-01
  5             8             1             0.324980E+00  0.118969E+00
  3             12            1             0.230760E+00  0.117415E+00
  3             13            1             0.230760E+00  0.117415E+00
  3             8             1             0.273040E+00  0.174152E+00
  4             17            1             0.285040E+00  0.149399E+00
  4             18            1             0.285040E+00  0.149399E+00
  4             19            1             0.285040E+00  0.149399E+00
  12            17            1             0.250000E+00  0.627612E-01
  12            18            1             0.250000E+00  0.627612E-01
  12            19            1             0.250000E+00  0.627612E-01
  13            17            1             0.250000E+00  0.627612E-01
  13            18            1             0.250000E+00  0.627612E-01
  13            19            1             0.250000E+00  0.627612E-01

[ dihedrals ]
; i             j             k             l             func          phi0 (deg)    kphi (kJ/mol)  n
  9             6             2             1             1             0.0000        0.2750         3
  9             6             2             3             1             0.0000        0.0000         1
  10            6             2             1             1             0.0000        0.2750         3
  10            6             2             3             1             0.0000        0.0000         1
```

11	6	2	1	1	0.0000	0.2750	3
11	6	2	3	1	0.0000	0.0000	1
6	2	1	5	1	180.0000	6.2750	2
6	2	1	14	1	180.0000	6.2750	2
3	2	1	5	1	180.0000	6.2750	2
3	2	1	14	1	180.0000	6.2750	2
2	1	5	4	1	180.0000	22.4900	2
2	1	5	15	1	180.0000	22.4900	2
14	1	5	4	1	180.0000	22.4900	2
14	1	5	15	1	180.0000	22.4900	2
1	5	4	3	1	180.0000	6.2750	2
1	5	4	7	1	180.0000	6.2750	2
15	5	4	3	1	180.0000	6.2750	2
15	5	4	7	1	180.0000	6.2750	2
5	4	3	2	1	180.0000	9.7300	2
5	4	3	16	1	180.0000	9.7300	2
7	4	3	2	1	180.0000	9.7300	2
7	4	3	16	1	180.0000	9.7300	2
4	3	2	6	1	180.0000	9.7300	2
4	3	2	1	1	180.0000	9.7300	2
16	3	2	6	1	180.0000	9.7300	2
16	3	2	1	1	180.0000	9.7300	2
5	4	7	12	1	0.0000	0.2750	3
5	4	7	13	1	0.0000	0.2750	3
5	4	7	8	1	0.0000	-2.8800	1
5	4	7	8	1	180.0000	2.2150	2
5	4	7	8	1	0.0000	0.4385	3
3	4	7	12	1	0.0000	0.0000	1
3	4	7	13	1	0.0000	0.0000	1
3	4	7	8	1	0.0000	-1.2300	1
4	7	8	17	1	0.0000	0.0000	1
4	7	8	18	1	0.0000	0.0000	1
4	7	8	19	1	0.0000	0.0000	1
12	7	8	17	1	0.0000	0.6655	3
12	7	8	18	1	0.0000	0.6655	3
12	7	8	19	1	0.0000	0.6655	3
13	7	8	17	1	0.0000	0.6655	3
13	7	8	18	1	0.0000	0.6655	3
13	7	8	19	1	0.0000	0.6655	3
4	5	15	1	1	180.0000	4.6000	2
15	5	4	1	1	180.0000	4.6000	2
5	1	14	2	1	180.0000	4.6000	2
14	1	5	2	1	180.0000	4.6000	2
16	3	2	4	1	180.0000	4.6000	2
2	3	16	4	1	180.0000	4.6000	2
7	4	5	3	1	180.0000	4.1850	2
5	4	7	3	1	180.0000	4.1850	2
6	2	1	3	1	180.0000	4.1850	2
3	2	1	6	1	180.0000	4.1850	2

[exclusions]

; i	j
9	6
10	6
11	6
6	2
2	1
1	5
5	4
4	3
3	2
3	16
5	15
1	14
4	7
7	12
7	13
7	8
8	17
8	18
8	19
2	5
2	14
5	14
1	3
1	6
3	6
2	4
2	16
4	16
3	5
3	7
5	7
1	4
1	15
4	15
2	9
2	10
2	11
9	10
9	11
10	11
4	8

```
  4             12
  4             13
  8             12
  8             13
  12            13
  7             17
  7             18
  7             19
  17            18
  17            19
  18            19
  9             1
  9             3
  10            1
  10            3
  11            1
  11            3
  6             5
  6             14
  3             14
  2             15
  14            4
  14            15
  1             7
  15            3
  15            7
  5             16
  7             2
  7             16
  4             6
  16            6
  16            1
  5             12
  5             13
  5             8
  3             12
  3             13
  3             8
  4             17
  4             18
  4             19
  12            17
  12            18
  12            19
  13            17
  13            18
  13            19


[ moleculetype ]
; name          nrexcl
  ntf2          3

[ atoms ]
; nr            type            resnr           residue         atom            cgnr            charge
  1             c               1               ntf2            c               1               0.3500
  2             f               1               ntf2            f               2               -0.1600
  3             f               1               ntf2            f               3               -0.1600
  4             s               1               ntf2            s               4               1.0200
  5             o               1               ntf2            o               5               -0.5300
  6             f               1               ntf2            f               6               -0.1600
  7             o               1               ntf2            o               7               -0.5300
  8             n               1               ntf2            n               8               -0.6600
  9             s               1               ntf2            s               9               1.0200
  10            o               1               ntf2            o               10              -0.5300
  11            o               1               ntf2            o               11              -0.5300
  12            c               1               ntf2            c               12              0.3500
  13            f               1               ntf2            f               13              -0.1600
  14            f               1               ntf2            f               14              -0.1600
  15            f               1               ntf2            f               15              -0.1600

[ bonds ]
; i             j               func            b0 (nm)         kb (kJ/mol/nm2)
  1             2               1               0.132300E+00    0.369700E+06
  1             3               1               0.132300E+00    0.369700E+06
  1             6               1               0.132300E+00    0.369700E+06
  1             4               1               0.181800E+00    0.197000E+06
  4             5               1               0.144200E+00    0.533100E+06
  4             7               1               0.144200E+00    0.533100E+06
  4             8               1               0.157000E+00    0.311300E+06
  8             9               1               0.157000E+00    0.311300E+06
  9             10              1               0.144200E+00    0.533100E+06
  9             11              1               0.144200E+00    0.533100E+06
  9             12              1               0.181800E+00    0.197000E+06
  12            13              1               0.132300E+00    0.369700E+06
  12            14              1               0.132300E+00    0.369700E+06
  12            15              1               0.132300E+00    0.369700E+06

[ angles ]
; i             j               k               func            th0 (deg)       kth (kJ/mol/rad2)
```

2	1	3	1	0.107100E+03	0.781000E+03
2	1	4	1	0.111800E+03	0.694000E+03
2	1	6	1	0.107100E+03	0.781000E+03
3	1	4	1	0.111800E+03	0.694000E+03
3	1	6	1	0.107100E+03	0.781000E+03
4	1	6	1	0.111800E+03	0.694000E+03
1	4	5	1	0.102600E+03	0.870000E+03
1	4	7	1	0.102600E+03	0.870000E+03
1	4	8	1	0.100200E+03	0.816000E+03
5	4	7	1	0.118500E+03	0.969000E+03
5	4	8	1	0.113600E+03	0.789000E+03
7	4	8	1	0.113600E+03	0.789000E+03
4	8	9	1	0.125600E+03	0.671000E+03
8	9	10	1	0.113600E+03	0.789000E+03
8	9	11	1	0.113600E+03	0.789000E+03
8	9	12	1	0.100200E+03	0.816000E+03
10	9	11	1	0.118500E+03	0.969000E+03
10	9	12	1	0.102600E+03	0.870000E+03
11	9	12	1	0.102600E+03	0.870000E+03
9	12	13	1	0.111800E+03	0.694000E+03
9	12	14	1	0.111800E+03	0.694000E+03
9	12	15	1	0.111800E+03	0.694000E+03
13	12	14	1	0.107100E+03	0.781000E+03
13	12	15	1	0.107100E+03	0.781000E+03
14	12	15	1	0.107100E+03	0.781000E+03

[dihedrals]

; i	j	k	l	func	phi0 (deg)	kphi (kJ/mol)	n
2	1	4	5	1	0.0000	0.7255	3
2	1	4	7	1	0.0000	0.7255	3
2	1	4	8	1	0.0000	0.6610	3
3	1	4	5	1	0.0000	0.7255	3
3	1	4	7	1	0.0000	0.7255	3
3	1	4	8	1	0.0000	0.6610	3
6	1	4	5	1	0.0000	0.7255	3
6	1	4	7	1	0.0000	0.7255	3
6	1	4	8	1	0.0000	0.6610	3
1	4	8	9	1	0.0000	32.3165	1
1	4	8	9	1	0.0000	7.2021	2
1	4	8	9	1	0.0000	-1.3134	3
1	4	8	9	1	0.0000	-0.5525	4
1	4	8	9	1	0.0000	0.2082	7
1	4	8	9	1	0.0000	0.1549	8
1	4	8	9	1	90.0000	1.2131	1
1	4	8	9	1	90.0000	-1.5370	3
1	4	8	9	1	90.0000	0.3973	4
1	4	8	9	1	90.0000	-0.2391	5
1	4	8	9	1	90.0000	-0.3251	6
1	4	8	9	1	90.0000	0.1928	8
4	8	9	12	1	0.0000	32.3165	1
4	8	9	12	1	0.0000	7.2021	2
4	8	9	12	1	0.0000	-1.3134	3
4	8	9	12	1	0.0000	-0.5525	4
4	8	9	12	1	0.0000	0.2082	7
4	8	9	12	1	0.0000	0.1549	8
4	8	9	12	1	90.0000	1.2131	1
4	8	9	12	1	90.0000	-1.5370	3
4	8	9	12	1	90.0000	0.3973	4
4	8	9	12	1	90.0000	-0.2391	5
4	8	9	12	1	90.0000	-0.3251	6
4	8	9	12	1	90.0000	0.1928	8
8	9	12	13	1	0.0000	0.6610	3
8	9	12	14	1	0.0000	0.6610	3
8	9	12	15	1	0.0000	0.6610	3
10	9	12	13	1	0.0000	0.7255	3
10	9	12	14	1	0.0000	0.7255	3
10	9	12	15	1	0.0000	0.7255	3
11	9	12	13	1	0.0000	0.7255	3
11	9	12	14	1	0.0000	0.7255	3
11	9	12	15	1	0.0000	0.7255	3

[exclusions]

; i	j
1	2
1	3
1	6
1	4
4	5
4	7
4	8
8	9
9	10
9	11
9	12
12	13
12	14
12	15
2	3
2	4
2	6
3	4
3	6
4	6

```
  1             5
  1             7
  1             8
  5             7
  5             8
  7             8
  4             9
  8             10
  8             11
  8             12
  10            11
  10            12
  11            12
  9             13
  9             14
  9             15
  13            14
  13            15
  14            15
  2             5
  2             7
  2             8
  3             5
  3             7
  3             8
  6             5
  6             7
  6             8
  1             9
  5             9
  7             9
  4             10
  4             11
  4             12
  8             13
  8             14
  8             15
  10            13
  10            14
  10            15
  11            13
  11            14
  11            15



[ system ]
; name
  C2MIM-NTF2 according to Ludwig et al.

[ molecules ]
; name          number
  c2            1686
  ntf2          1686
  alu           4845
  oxy           6885
  ohy           765
```

Ludwig – Geometric (LG)

```
[ defaults ]
; nbfunc        comb-rule       gen-pairs       fudgeLJ         fudgeQQ
  1             3               yes             1.0             1.0

[ atomtypes ]
; name          mass            charge          ptype           sig             eps
  cw            12.01000        -0.13000        A               0.30175         0.20502
  na            14.01000        0.15000         A               0.32500         0.71128
  cr            12.01000        -0.11000        A               0.21300         0.43933
  c1            12.01000        -0.17000        A               0.35000         0.27614
  ce            12.01000        -0.05000        A               0.35000         0.27614
  h1            1.00800         0.13000         A               0.25000         0.12552
  hb            1.00800         0.21000         A               0.20570         0.08787
  ha            1.00800         0.21000         A               0.14520         0.18828
  hc            1.00800         0.06000         A               0.25000         0.12552
  f             19.00000        -0.16000        A               0.26550         0.06651
  c             12.01000        0.35000         A               0.31500         0.08282
  o             16.00000        -0.53000        A               0.34632         0.26353
  s             32.07000        1.02000         A               0.40825         0.31373
  n             14.01000        -0.66000        A               0.32500         0.21334
  al            26.98200        1.57500         A               0.42712         5.65390E-06
  os            16.00000        -1.05000        A               0.31655         0.65019
  oh            16.00000        -0.95000        A               0.31655         0.65019
  ho            1.00800         0.42500         A               0.00000         0.00000

[ nonbond_params ]
; i             j               func            sig             eps
  al            al              1               0.42712         5.65390E-06
  al            os              1               0.371835        0.001917318
  al            oh              1               0.371835        0.001917318
  al            ho              1               0.21356         0.000000
  os            os              1               0.31655         0.65019
  os            oh              1               0.31655         0.65019
  os            ho              1               0.158275        0.000000
  oh            oh              1               0.31655         0.65019
  oh            ho              1               0.158275        0.000000
  ho            ho              1               0.000000        0.000000


[ moleculetype ]
; name          nrexcl
  alu           1

[ atoms ]
; nr            type            resnr           residue         atom            cgnr            charge
  1             al              1               alu             al              1               1.57500


[ moleculetype ]
; name          nrexcl
  oxy           1

[ atoms ]
; nr            type            resnr           residue         atom            cgnr            charge
  1             os              1               oxy             os              1               -1.05000


[ moleculetype ]
; name          nrexcl
  ohy           2

[ atoms ]
; nr            type            resnr           residue         atom            cgnr            charge
  1             oh              1               ohy             oh              1               -0.95000
  2             ho              1               ohy             ho              2               0.42500

[ bonds ]
; i             j               func            b0 (nm)         kb (kJ/mol/nm2)
  2             1               1               0.10000E+00     0.4637001E+06


[ moleculetype ]
; name          nrexcl
  c2            3

[ atoms ]
; nr            type            resnr           residue         atom            cgnr            charge
  1             cw              1               c2              cw              1               -0.1300
```

2	na	1	c2	na	2	0.1500
3	cr	1	c2	cr	3	-0.1100
4	na	1	c2	na	4	0.1500
5	cw	1	c2	cw	5	-0.1300
6	c1	1	c2	c1	6	-0.1700
7	c1	1	c2	c1	7	-0.1700
8	ce	1	c2	ce	8	-0.0500
9	h1	1	c2	h1	9	0.1300
10	h1	1	c2	h1	10	0.1300
11	h1	1	c2	h1	11	0.1300
12	h1	1	c2	h1	12	0.1300
13	h1	1	c2	h1	13	0.1300
14	hb	1	c2	hb	14	0.2100
15	hb	1	c2	hb	15	0.2100
16	ha	1	c2	ha	16	0.2100
17	hc	1	c2	hc	17	0.0600
18	hc	1	c2	hc	18	0.0600
19	hc	1	c2	hc	19	0.0600

[bonds]

; i	j	func	b0 (nm)	kb (kJ/mol/nm2)
6	2	1	0.146600E+00	0.141000E+06
2	1	1	0.137800E+00	0.178700E+06
1	5	1	0.134100E+00	0.217600E+06
5	4	1	0.137800E+00	0.178700E+06
4	3	1	0.131500E+00	0.199600E+06
3	2	1	0.131500E+00	0.199600E+06
4	7	1	0.146600E+00	0.141000E+06
7	8	1	0.152900E+00	0.112100E+06

[constraints]

; i	j	func	b0 (nm)
9	6	1	0.109000E+00
10	6	1	0.109000E+00
11	6	1	0.109000E+00
3	16	1	0.108000E+00
5	15	1	0.108000E+00
1	14	1	0.108000E+00
7	12	1	0.109000E+00
7	13	1	0.109000E+00
8	17	1	0.109000E+00
8	18	1	0.109000E+00
8	19	1	0.109000E+00

[angles]

; i	j	k	func	th0 (deg)	kth (kJ/mol/rad2)
2	1	5	1	0.107100E+03	0.292600E+03
2	1	14	1	0.122000E+03	0.146300E+03
5	1	14	1	0.130900E+03	0.146300E+03
1	2	3	1	0.108000E+03	0.292600E+03
1	2	6	1	0.125600E+03	0.292600E+03
3	2	6	1	0.126400E+03	0.292600E+03
2	3	4	1	0.109800E+03	0.292600E+03
2	3	16	1	0.125100E+03	0.146300E+03
4	3	16	1	0.125100E+03	0.146300E+03
3	4	5	1	0.108000E+03	0.292600E+03
3	4	7	1	0.126400E+03	0.292600E+03
5	4	7	1	0.125600E+03	0.292600E+03
1	5	4	1	0.107100E+03	0.292600E+03
1	5	15	1	0.130900E+03	0.146300E+03
4	5	15	1	0.122000E+03	0.146300E+03
2	6	9	1	0.110700E+03	0.313200E+03
2	6	10	1	0.110700E+03	0.313200E+03
2	6	11	1	0.110700E+03	0.313200E+03
9	6	10	1	0.107800E+03	0.276200E+03
9	6	11	1	0.107800E+03	0.276200E+03
10	6	11	1	0.107800E+03	0.276200E+03
4	7	8	1	0.112700E+03	0.418400E+03
4	7	12	1	0.110700E+03	0.313200E+03
4	7	13	1	0.110700E+03	0.313200E+03
8	7	12	1	0.110700E+03	0.313200E+03
8	7	13	1	0.110700E+03	0.313200E+03
12	7	13	1	0.107800E+03	0.276200E+03
7	8	17	1	0.110700E+03	0.313200E+03
7	8	18	1	0.110700E+03	0.313200E+03
7	8	19	1	0.110700E+03	0.313200E+03
17	8	18	1	0.107800E+03	0.276200E+03
17	8	19	1	0.107800E+03	0.276200E+03
18	8	19	1	0.107800E+03	0.276200E+03

[pairs]

; i	j	func	sig	eps
9	1	1	0.274660E+00	0.802092E-01
9	3	1	0.230760E+00	0.117415E+00
10	1	1	0.274660E+00	0.802092E-01
10	3	1	0.230760E+00	0.117415E+00
11	1	1	0.274660E+00	0.802092E-01
11	3	1	0.230760E+00	0.117415E+00
6	5	1	0.324980E+00	0.118969E+00
6	14	1	0.268320E+00	0.778837E-01
3	14	1	0.209320E+00	0.982359E-01
2	15	1	0.258560E+00	0.124997E+00
14	4	1	0.258560E+00	0.124997E+00

14	15	1	0.205700E+00	0.439330E-01
1	7	1	0.324980E+00	0.118969E+00
15	3	1	0.209320E+00	0.982359E-01
15	7	1	0.268320E+00	0.778837E-01
5	16	1	0.209320E+00	0.982359E-01
7	2	1	0.337270E+00	0.221593E+00
7	16	1	0.225430E+00	0.114010E+00
4	6	1	0.337270E+00	0.221593E+00
16	6	1	0.225430E+00	0.114010E+00
16	1	1	0.209320E+00	0.982359E-01
5	12	1	0.274660E+00	0.802092E-01
5	13	1	0.274660E+00	0.802092E-01
5	8	1	0.324980E+00	0.118969E+00
3	12	1	0.230760E+00	0.117415E+00
3	13	1	0.230760E+00	0.117415E+00
3	8	1	0.273040E+00	0.174152E+00
4	17	1	0.285040E+00	0.149399E+00
4	18	1	0.285040E+00	0.149399E+00
4	19	1	0.285040E+00	0.149399E+00
12	17	1	0.250000E+00	0.627612E-01
12	18	1	0.250000E+00	0.627612E-01
12	19	1	0.250000E+00	0.627612E-01
13	17	1	0.250000E+00	0.627612E-01
13	18	1	0.250000E+00	0.627612E-01
13	19	1	0.250000E+00	0.627612E-01

[dihedrals]

; i	j	k	l	func	phi0 (deg)	kphi (kJ/mol)	n
9	6	2	1	1	0.0000	0.2750	3
9	6	2	3	1	0.0000	0.0000	1
10	6	2	1	1	0.0000	0.2750	3
10	6	2	3	1	0.0000	0.0000	1
11	6	2	1	1	0.0000	0.2750	3
11	6	2	3	1	0.0000	0.0000	1
6	2	1	5	1	180.0000	6.2750	2
6	2	1	14	1	180.0000	6.2750	2
3	2	1	5	1	180.0000	6.2750	2
3	2	1	14	1	180.0000	6.2750	2
2	1	5	4	1	180.0000	22.4900	2
2	1	5	15	1	180.0000	22.4900	2
14	1	5	4	1	180.0000	22.4900	2
14	1	5	15	1	180.0000	22.4900	2
1	5	4	3	1	180.0000	6.2750	2
1	5	4	7	1	180.0000	6.2750	2
15	5	4	3	1	180.0000	6.2750	2
15	5	4	7	1	180.0000	6.2750	2
5	4	3	2	1	180.0000	9.7300	2
5	4	3	16	1	180.0000	9.7300	2
7	4	3	2	1	180.0000	9.7300	2
7	4	3	16	1	180.0000	9.7300	2
4	3	2	6	1	180.0000	9.7300	2
4	3	2	1	1	180.0000	9.7300	2
16	3	2	6	1	180.0000	9.7300	2
16	3	2	1	1	180.0000	9.7300	2
5	4	7	12	1	0.0000	0.2750	3
5	4	7	13	1	0.0000	0.2750	3
5	4	7	8	1	0.0000	-2.8800	1
5	4	7	8	1	180.0000	2.2150	2
5	4	7	8	1	0.0000	0.4385	3
3	4	7	12	1	0.0000	0.0000	1
3	4	7	13	1	0.0000	0.0000	1
3	4	7	8	1	0.0000	-1.2300	1
4	7	8	17	1	0.0000	0.0000	1
4	7	8	18	1	0.0000	0.0000	1
4	7	8	19	1	0.0000	0.0000	1
12	7	8	17	1	0.0000	0.6655	3
12	7	8	18	1	0.0000	0.6655	3
12	7	8	19	1	0.0000	0.6655	3
13	7	8	17	1	0.0000	0.6655	3
13	7	8	18	1	0.0000	0.6655	3
13	7	8	19	1	0.0000	0.6655	3
4	5	15	1	1	180.0000	4.6000	2
15	5	4	1	1	180.0000	4.6000	2
5	1	14	2	1	180.0000	4.6000	2
14	1	5	2	1	180.0000	4.6000	2
16	3	2	4	1	180.0000	4.6000	2
2	3	16	4	1	180.0000	4.6000	2
7	4	5	3	1	180.0000	4.1850	2
5	4	7	3	1	180.0000	4.1850	2
6	2	1	3	1	180.0000	4.1850	2
3	2	1	6	1	180.0000	4.1850	2

[exclusions]

; i	j
9	6
10	6
11	6
6	2
2	1
1	5
5	4
4	3
3	2

```
  3             16
  5             15
  1             14
  4             7
  7             12
  7             13
  7             8
  8             17
  8             18
  8             19
  2             5
  2             14
  5             14
  1             3
  1             6
  3             6
  2             4
  2             16
  4             16
  3             5
  3             7
  5             7
  1             4
  1             15
  4             15
  2             9
  2             10
  2             11
  9             10
  9             11
  10            11
  4             8
  4             12
  4             13
  8             12
  8             13
  12            13
  7             17
  7             18
  7             19
  17            18
  17            19
  18            19
  9             1
  9             3
  10            1
  10            3
  11            1
  11            3
  6             5
  6             14
  3             14
  2             15
  14            4
  14            15
  1             7
  15            3
  15            7
  5             16
  7             2
  7             16
  4             6
  16            6
  16            1
  5             12
  5             13
  5             8
  3             12
  3             13
  3             8
  4             17
  4             18
  4             19
  12            17
  12            18
  12            19
  13            17
  13            18
  13            19


[ moleculetype ]
; name          nrexcl
  ntf2          3

[ atoms ]
; nr            type            resnr           residue         atom            cgnr            charge
  1             c               1               ntf2            c               1               0.3500
  2             f               1               ntf2            f               2               -0.1600
  3             f               1               ntf2            f               3               -0.1600
```

4	s	1	ntf2	s	4	1.0200
5	o	1	ntf2	o	5	-0.5300
6	f	1	ntf2	f	6	-0.1600
7	o	1	ntf2	o	7	-0.5300
8	n	1	ntf2	n	8	-0.6600
9	s	1	ntf2	s	9	1.0200
10	o	1	ntf2	o	10	-0.5300
11	o	1	ntf2	o	11	-0.5300
12	c	1	ntf2	c	12	0.3500
13	f	1	ntf2	f	13	-0.1600
14	f	1	ntf2	f	14	-0.1600
15	f	1	ntf2	f	15	-0.1600

[bonds]

; i	j	func	b0 (nm)	kb (kJ/mol/nm2)
1	2	1	0.132300E+00	0.369700E+06
1	3	1	0.132300E+00	0.369700E+06
1	6	1	0.132300E+00	0.369700E+06
1	4	1	0.181800E+00	0.197000E+06
4	5	1	0.144200E+00	0.533100E+06
4	7	1	0.144200E+00	0.533100E+06
4	8	1	0.157000E+00	0.311300E+06
8	9	1	0.157000E+00	0.311300E+06
9	10	1	0.144200E+00	0.533100E+06
9	11	1	0.144200E+00	0.533100E+06
9	12	1	0.181800E+00	0.197000E+06
12	13	1	0.132300E+00	0.369700E+06
12	14	1	0.132300E+00	0.369700E+06
12	15	1	0.132300E+00	0.369700E+06

[angles]

; i	j	k	func	th0 (deg)	kth (kJ/mol/rad2)
2	1	3	1	0.107100E+03	0.781000E+03
2	1	4	1	0.111800E+03	0.694000E+03
2	1	6	1	0.107100E+03	0.781000E+03
3	1	4	1	0.111800E+03	0.694000E+03
3	1	6	1	0.107100E+03	0.781000E+03
4	1	6	1	0.111800E+03	0.694000E+03
1	4	5	1	0.102600E+03	0.870000E+03
1	4	7	1	0.102600E+03	0.870000E+03
1	4	8	1	0.100200E+03	0.816000E+03
5	4	7	1	0.118500E+03	0.969000E+03
5	4	8	1	0.113600E+03	0.789000E+03
7	4	8	1	0.113600E+03	0.789000E+03
4	8	9	1	0.125600E+03	0.671000E+03
8	9	10	1	0.113600E+03	0.789000E+03
8	9	11	1	0.113600E+03	0.789000E+03
8	9	12	1	0.100200E+03	0.816000E+03
10	9	11	1	0.118500E+03	0.969000E+03
10	9	12	1	0.102600E+03	0.870000E+03
11	9	12	1	0.102600E+03	0.870000E+03
9	12	13	1	0.111800E+03	0.694000E+03
9	12	14	1	0.111800E+03	0.694000E+03
9	12	15	1	0.111800E+03	0.694000E+03
13	12	14	1	0.107100E+03	0.781000E+03
13	12	15	1	0.107100E+03	0.781000E+03
14	12	15	1	0.107100E+03	0.781000E+03

[dihedrals]

; i	j	k	l	func	phi0 (deg)	kphi (kJ/mol)	n
2	1	4	5	1	0.0000	0.7255	3
2	1	4	7	1	0.0000	0.7255	3
2	1	4	8	1	0.0000	0.6610	3
3	1	4	5	1	0.0000	0.7255	3
3	1	4	7	1	0.0000	0.7255	3
3	1	4	8	1	0.0000	0.6610	3
6	1	4	5	1	0.0000	0.7255	3
6	1	4	7	1	0.0000	0.7255	3
6	1	4	8	1	0.0000	0.6610	3
1	4	8	9	1	0.0000	32.3165	1
1	4	8	9	1	0.0000	7.2021	2
1	4	8	9	1	0.0000	-1.3134	3
1	4	8	9	1	0.0000	-0.5525	4
1	4	8	9	1	0.0000	0.2082	7
1	4	8	9	1	0.0000	0.1549	8
1	4	8	9	1	90.0000	1.2131	1
1	4	8	9	1	90.0000	-1.5370	3
1	4	8	9	1	90.0000	0.3973	4
1	4	8	9	1	90.0000	-0.2391	5
1	4	8	9	1	90.0000	-0.3251	6
1	4	8	9	1	90.0000	0.1928	8
4	8	9	12	1	0.0000	32.3165	1
4	8	9	12	1	0.0000	7.2021	2
4	8	9	12	1	0.0000	-1.3134	3
4	8	9	12	1	0.0000	-0.5525	4
4	8	9	12	1	0.0000	0.2082	7
4	8	9	12	1	0.0000	0.1549	8
4	8	9	12	1	90.0000	1.2131	1
4	8	9	12	1	90.0000	-1.5370	3
4	8	9	12	1	90.0000	0.3973	4
4	8	9	12	1	90.0000	-0.2391	5
4	8	9	12	1	90.0000	-0.3251	6
4	8	9	12	1	90.0000	0.1928	8

```
  8             9             12            13            1             0.0000        0.6610        3
  8             9             12            14            1             0.0000        0.6610        3
  8             9             12            15            1             0.0000        0.6610        3
  10            9             12            13            1             0.0000        0.7255        3
  10            9             12            14            1             0.0000        0.7255        3
  10            9             12            15            1             0.0000        0.7255        3
  11            9             12            13            1             0.0000        0.7255        3
  11            9             12            14            1             0.0000        0.7255        3
  11            9             12            15            1             0.0000        0.7255        3

[ exclusions ]
; i             j
  1             2
  1             3
  1             6
  1             4
  4             5
  4             7
  4             8
  8             9
  9             10
  9             11
  9             12
  12            13
  12            14
  12            15
  2             3
  2             4
  2             6
  3             4
  3             6
  4             6
  1             5
  1             7
  1             8
  5             7
  5             8
  7             8
  4             9
  8             10
  8             11
  8             12
  10            11
  10            12
  11            12
  9             13
  9             14
  9             15
  13            14
  13            15
  14            15
  2             5
  2             7
  2             8
  3             5
  3             7
  3             8
  6             5
  6             7
  6             8
  1             9
  5             9
  7             9
  4             10
  4             11
  4             12
  8             13
  8             14
  8             15
  10            13
  10            14
  10            15
  11            13
  11            14
  11            15



[ system ]
; name
  C2MIM-NTF2 according to Ludwig et al.

[ molecules ]
; name          number
  c2            1686
  ntf2          1686
  alu           4845
  oxy           6885
  ohy           765
```

Maginn – Lorentz-Berthelot (ML)

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

[ atomtypes ]
; C2MIM
; name          mass            charge          ptype           sig             eps
  CPH1          12.0112         -0.134873       A               0.3207          0.2092
  CPH2          12.0112         -0.091215       A               0.3207          0.2092
  NR1           14.0064         0.059417        A               0.3296          0.8368
  HR3           1.0080          0.209995        A               0.2616          0.0326352
  HR1           1.0080          0.218877        A               0.1604          0.192464
  CN7B          12.0112         -0.250840       A               0.4054          0.08368
  HN7           1.0080          0.145165        A               0.2352          0.092048
  CT2           12.0112         0.253926        A               0.3875          0.23012
  CT3           12.0112         -0.104555       A               0.3875          0.23012
; NTF2
; name          mass            charge          ptype           sig             eps
  NTF2          14.0064         -0.660000       A               0.325           0.71128
  STF2          32.0655         1.020000        A               0.355           1.046
  CTF2          12.0112         0.350000        A               0.35            0.276144
  OTF2          15.9994         -0.530000       A               0.296           0.87864
  FTF2          18.9984         -0.160000       A               0.295           0.221752
; Alumina
; name          mass            charge          ptype           sig             eps
  AL            26.98200        1.57500         A               0.42712         5.65390E-06
  OS            16.00000        -1.05000        A               0.31655         0.65019
  OH            16.00000        -0.95000        A               0.31655         0.65019
  HO            1.00800         0.42500         A               0.00000         0.00000

[ bondtypes ]
; C2MIM
; i             j               func            b0 (nm)         kb (kJ/mol/nm2)
  CN7B          NR1             1               0.14762         0.092048E+06
  CPH1          NR1             1               0.13819         0.16736E+06
  CPH2          NR1             1               0.13366         0.16736E+06
  CPH1          CPH1            1               0.1361          0.171544E+06
  CPH2          HR1             1               0.10779         0.142256E+06
  CPH1          HR3             1               0.10775         0.152716E+06
  CN7B          HN7             1               0.10899         0.129286E+06
  CT3           HN7             1               0.10935         0.134725E+06
  CN7B          CT3             1               0.15308         0.08368E+06
; NTF2
; i             j               func            b0 (nm)         kb (kJ/mol/nm2)
  CTF2          FTF2            1               0.1323          0.18485E+06
  CTF2          STF2            1               0.1818          0.0985001E+06
  STF2          OTF2            1               0.1442          0.26655E+06
  NTF2          STF2            1               0.157           0.15565E+06

[ angletypes ]
; C2MIM
; i             j               k               func            th0 (deg)       kth (kJ/mol/rad2)
  CT2           CN7B            NR1             1               112.34          0.58576E+03
  CPH1          NR1             CPH2            1               108.25          0.54392E+03
  HN7           CN7B            NR1             1               109.41          0.12552E+03
  HR1           CPH2            NR1             1               125.44          0.1046E+03
  NR1           CPH1            CPH1            1               107.28          0.54392E+03
  NR1           CPH2            NR1             1               109.11          0.54392E+03
  HR3           CPH1            CPH1            1               130.74          0.1046E+03
  NR1           CPH1            HR3             1               122.04          0.1046E+03
  HN7           CN7B            HN7             1               108.44          0.148532E+03
  HN7           CN7B            CT2             1               111.68          0.139746E+03
  HN7           CT2             CN7B            1               109.13          0.139746E+03
  CN7B          CT2             CT2             1               111.50          0.244136E+03
  CT2           CT2             CT3             1               112.34          0.242672E+03
  HN7           CT2             HN7             1               106.13          0.148532E+03
  HN7           CT3             HN7             1               107.24          0.148532E+03
  CT2           CT2             HN7             1               108.43          0.110876E+03
  CT3           CT2             HN7             1               109.47          0.144766E+03
  CT2           CT3             HN7             1               111.62          0.144766E+03
  CN7B          NR1             CPH2            1               125.75          0.54392E+03
  CN7B          NR1             CPH1            1               125.67          0.54392E+03
  CT3           CN7B            NR1             1               112.34          0.58576E+03
  HN7           CN7B            CT3             1               111.68          0.139746E+03
  HN7           CT3             CN7B            1               109.13          0.139746E+03
  CT2           CT2             CT2             1               114.27          0.244136E+03
; NTF2
; i             j               k               func            th0 (deg)       kth (kJ/mol/rad2)
  FTF2          CTF2            FTF2            1               107.10          0.390493E+03
  STF2          CTF2            FTF2            1               111.80          0.346979E+03
  CTF2          STF2            OTF2            1               102.60          0.43501E+03
  OTF2          STF2            OTF2            1               118.50          0.484507E+03
  OTF2          STF2            NTF2            1               113.60          0.39543E+03
  CTF2          STF2            NTF2            1               100.20          0.407982E+03
  STF2          NTF2            STF2            1               125.60          0.335515E+03
```

```
[ dihedraltypes ]
; C2MIM
; i          j          k          l          func       phi0 (deg)     kphi (kJ/mol)  n
  CPH2       NR1        CPH1       CPH1       1          180            58.576         2
  NR1        CPH1       CPH1       NR1        1          180            58.576         2
  NR1        CPH2       NR1        CPH1       1          180            58.576         2
  HR1        CPH2       NR1        CPH1       1          180            12.552         2
  HR3        CPH1       CPH1       HR3        1          180            8.368          2
  CPH1       CPH1       NR1        CN7B       1          0              0              1
  HR3        CPH1       NR1        CPH2       1          180            12.552         2
  NR1        CPH1       CPH1       HR3        1          180            12.552         2
  NR1        CPH2       NR1        CN7B       1          180            0              2
  HR1        CPH2       NR1        CN7B       1          180            0              2
  HR3        CPH1       NR1        CN7B       1          180            0              2
  CPH2       NR1        CN7B       HN7        1          180            0.81588        2
  CPH1       NR1        CN7B       HN7        1          0              0              3
  CPH2       NR1        CN7B       CT2        1          180            0.4184         3
  CPH1       NR1        CN7B       CT2        1          0              0.8368         4
  NR1        CN7B       CT2        CT2        1          0              0              3
  HN7        CT2        CT3        HN7        1          0              0.66944        3
  CT2        CT2        CT3        HN7        1          0              0.66944        3
  NR1        CN7B       CT2        HN7        1          0              0              3
  CN7B       CT2        CT2        CT3        1          0              0.6276         1
  HN7        CN7B       CT2        HN7        1          0              0.81588        3
  HN7        CN7B       CT2        CT2        1          0              0.81588        3
  HN7        CT2        CT2        HN7        1          0              0.81588        3
  CN7B       CT2        CT2        HN7        1          0              0.81588        3
  HN7        CT2        CT2        CT3        1          0              0.81588        3
  CPH2       NR1        CN7B       CT3        1          180            0.4184         3
  CPH1       NR1        CN7B       CT3        1          0              0.8368         4
  NR1        CN7B       CT3        HN7        1          0              0              3
  HN7        CN7B       CT3        HN7        1          0              0.81588        3
  CT2        CT2        CT2        CT2        1          0              0.81588        3
  CT2        CT2        CT2        CT3        1          0              0.81588        3
  CN7B       CT2        CT2        CT2        1          0              0.81588        3
  CT2        CT2        CT2        HN7        1          0              0.81588        3
; C2MIM (impropers)
; i          j          k          l          func       xi0 (deg)      kxi (kJ/mol/rad2)
  CPH2       NR1        NR1        HR1        2          0              2.09200
  NR1        CPH1       CPH2       CN7B       2          0              2.51040
  CPH1       CPH1       NR1        HR3        2          0              2.09200
; NTF 2
; i          j          k          l          func       phi0 (deg)     kphi (kJ/mol)  n
  FTF2       CTF2       STF2       OTF2       1          0              0.725506       3
  STF2       NTF2       STF2       OTF2       1          0              -0.0075312     3
  FTF2       CTF2       STF2       NTF2       1          0              0.661072       3
  STF2       NTF2       STF2       CTF2       9          0              32.7729        1
  STF2       NTF2       STF2       CTF2       9          180            -10.4198       2
  STF2       NTF2       STF2       CTF2       9          0              -3.1949        3


[ moleculetype ]
; name       nrexcl
  alu        1

[ atoms ]
; nr         type       resnr      residue    name       cgnr       charge
  1          AL         1          alu        al         1          1.57500


[ moleculetype ]
; name       nrexcl
  oxy        1

[ atoms ]
; nr         type       resnr      residue    atom       cgnr       charge
  1          OS         1          oxy        os         1          -1.05000


[ moleculetype ]
; name       nrexcl
  ohy        2

[ atoms ]
; nr         type       resnr      residue    atom       cgnr       charge
  1          OH         1          ohy        oh         1          -0.95000
  2          HO         1          ohy        ho         2          0.42500

[ bonds ]
; i          j          func       b0 (nm)    kb (kJ/mol/nm2)
  2          1          1          0.10000    0.4637001E+06
```

```
[ moleculetype ]
; name          nrexcl
  c2            3

[ atoms ]
; nr            type          resnr         residue       name          cgnr          charge
  1             CPH1          1             c2            cw            1             -0.147177
  2             NR1           1             c2            na            2             0.193715
  3             CPH2          1             c2            cr            3             -0.091215
  4             NR1           1             c2            na            4             0.059417
  5             CPH1          1             c2            cw            5             -0.134873
  6             CN7B          1             c2            c1            6             -0.250840
  7             CN7B          1             c2            c1            7             0.103944
  8             CT3           1             c2            ce            8             -0.104555
  9             HN7           1             c2            h1            9             0.145165
  10            HN7           1             c2            h1            10            0.145165
  11            HN7           1             c2            h1            11            0.145165
  12            HN7           1             c2            h1            12            0.055550
  13            HN7           1             c2            h1            13            0.055550
  14            HR3           1             c2            hb            14            0.209995
  15            HR3           1             c2            hb            15            0.220374
  16            HR1           1             c2            ha            16            0.218877
  17            HN7           1             c2            hc            17            0.058581
  18            HN7           1             c2            hc            18            0.058581
  19            HN7           1             c2            hc            19            0.058581

[ bonds ]
; i             j
  6             2
  2             1
  1             5
  5             4
  4             3
  3             2
  4             7
  7             8
  9             6
  10            6
  11            6
  3             16
  5             15
  1             14
  7             12
  7             13
  8             17
  8             18
  8             19

[ angles ]
; i             j             k
  2             1             5
  2             1             14
  5             1             14
  1             2             3
  1             2             6
  3             2             6
  2             3             4
  2             3             16
  4             3             16
  3             4             5
  3             4             7
  5             4             7
  1             5             4
  1             5             15
  4             5             15
  2             6             9
  2             6             10
  2             6             11
  9             6             10
  9             6             11
  10            6             11
  4             7             8
  4             7             12
  4             7             13
  8             7             12
  8             7             13
  12            7             13
  7             8             17
  7             8             18
  7             8             19
  17            8             18
  17            8             19
  18            8             19

[ dihedrals ]
; i             j             k             l
  9             6             2             1
  9             6             2             3
  10            6             2             1
  10            6             2             3
  11            6             2             1
```

```
  11            6               2               3
  6             2               1               5
  6             2               1               14
  3             2               1               5
  3             2               1               14
  2             1               5               4
  2             1               5               15
  14            1               5               4
  14            1               5               15
  1             5               4               3
  1             5               4               7
  15            5               4               3
  15            5               4               7
  5             4               3               2
  5             4               3               16
  7             4               3               2
  7             4               3               16
  4             3               2               6
  4             3               2               1
  16            3               2               6
  16            3               2               1
  5             4               7               12
  5             4               7               13
  5             4               7               8
  3             4               7               12
  3             4               7               13
  3             4               7               8
  4             7               8               17
  4             7               8               18
  4             7               8               19
  12            7               8               17
  12            7               8               18
  12            7               8               19
  13            7               8               17
  13            7               8               18
  13            7               8               19
; impropers
  3             4               2               16              2
  4             5               3               7               2
  2             1               3               6               2
  1             5               2               14              2
  5             1               4               15              2

[ pairs ]
; i             j
  9             1
  9             3
  10            1
  10            3
  11            1
  11            3
  6             5
  6             14
  3             5
  3             14
  2             4
  2             15
  14            4
  14            15
  1             3
  1             7
  15            3
  15            7
  5             2
  5             16
  7             2
  7             16
  4             6
  4             1
  16            6
  16            1
  5             12
  5             13
  5             8
  3             12
  3             13
  3             8
  4             17
  4             18
  4             19
  12            17
  12            18
  12            19
  13            17
  13            18
  13            19



[ moleculetype ]
; name          nrexcl
```

```
  ntf2          3

[ atoms ]
; nr            type          resnr         residue       name          cgnr
  1             CTF2          1             ntf2          c             1
  2             FTF2          1             ntf2          f             2
  3             FTF2          1             ntf2          f             3
  4             STF2          1             ntf2          s             4
  5             OTF2          1             ntf2          o             5
  6             FTF2          1             ntf2          f             6
  7             OTF2          1             ntf2          o             7
  8             NTF2          1             ntf2          n             8
  9             STF2          1             ntf2          s             9
  10            OTF2          1             ntf2          o             10
  11            OTF2          1             ntf2          o             11
  12            CTF2          1             ntf2          c             12
  13            FTF2          1             ntf2          f             13
  14            FTF2          1             ntf2          f             14
  15            FTF2          1             ntf2          f             15

[ bonds ]
; i             j
  1             2
  1             3
  1             6
  1             4
  4             5
  4             7
  4             8
  8             9
  9             10
  9             11
  9             12
  12            13
  12            14
  12            15

[ angles ]
; i             j             k
  2             1             3
  2             1             4
  2             1             6
  3             1             4
  3             1             6
  4             1             6
  1             4             5
  1             4             7
  1             4             8
  5             4             7
  5             4             8
  7             4             8
  4             8             9
  8             9             10
  8             9             11
  8             9             12
  10            9             11
  10            9             12
  11            9             12
  9             12            13
  9             12            14
  9             12            15
  13            12            14
  13            12            15
  14            12            15

[ dihedrals ]
; i             j             k             l
; x             C             S             x
  2             1             4             8
  2             1             4             5
  2             1             4             7
  3             1             4             8
  3             1             4             5
  3             1             4             7
  6             1             4             8
  6             1             4             5
  6             1             4             7
  13            12            9             8
  14            12            9             8
  15            12            9             8
  13            12            9             10
  13            12            9             11
  14            12            9             10
  14            12            9             11
  15            12            9             10
; x             N             S             x
  4             8             9             12
  4             8             9             10
  4             8             9             11
  9             8             4             1
  9             8             4             5
  9             8             4             7
```

```
[ pairs ]
; i             j
  2             8
  2             5
  2             7
  3             8
  3             5
  3             7
  6             8
  6             5
  6             7
  13            8
  14            8
  15            8
  13            10
  13            11
  14            10
  14            11
  15            10
  4             12
  4             10
  4             11
  9             1
  9             5
  9             7
```

```
[ system ]
; name
  C2MIM-NTF2 according to Maginn et al.

[ molecules ]
; name          number
  c2            1686
  ntf2          1686
  alu           4845
  oxy           6885
  ohy           765
```

Maginn – Geometric (MG)

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

[ atomtypes ]
; C2MIM
; name          mass            charge          ptype           sig             eps
  CPH1          12.0112         -0.134873       A               0.3207          0.2092
  CPH2          12.0112         -0.091215       A               0.3207          0.2092
  NR1           14.0064         0.059417        A               0.3296          0.8368
  HR3           1.0080          0.209995        A               0.2616          0.0326352
  HR1           1.0080          0.218877        A               0.1604          0.192464
  CN7B          12.0112         -0.250840       A               0.4054          0.08368
  HN7           1.0080          0.145165        A               0.2352          0.092048
  CT2           12.0112         0.253926        A               0.3875          0.23012
  CT3           12.0112         -0.104555       A               0.3875          0.23012
; NTF2
; name          mass            charge          ptype           sig             eps
  NTF2          14.0064         -0.660000       A               0.325           0.71128
  STF2          32.0655         1.020000        A               0.355           1.046
  CTF2          12.0112         0.350000        A               0.35            0.276144
  OTF2          15.9994         -0.530000       A               0.296           0.87864
  FTF2          18.9984         -0.160000       A               0.295           0.221752
; Alumina
; name          mass            charge          ptype           sig             eps
  AL            26.98200        1.57500         A               0.42712         5.65390E-06
  OS            16.00000        -1.05000        A               0.31655         0.65019
  OH            16.00000        -0.95000        A               0.31655         0.65019
  HO            1.00800         0.42500         A               0.00000         0.00000

[ nonbond_params ]
; i             j               func            sig             eps
  CPH1          AL              1               0.864766        0.00108756
  CPH1          OS              1               0.798279        0.368809
  CPH1          OH              1               0.798279        0.368809
  CPH1          HO              1               0.566304        0
  CPH2          AL              1               0.864766        0.00108756
  CPH2          OS              1               0.798279        0.368809
  CPH2          OH              1               0.798279        0.368809
  CPH2          HO              1               0.566304        0
  NR1           AL              1               0.869897        0.00217513
  NR1           OS              1               0.803835        0.737617
  NR1           OH              1               0.803835        0.737617
  NR1           HO              1               0.574108        0
  HR3           AL              1               0.829892        0.000429553
  HR3           OS              1               0.760362        0.145668
  HR3           OH              1               0.760362        0.145668
  HR3           HO              1               0.511468        0
  HR1           AL              1               0.766499        0.00104315
  HR1           OS              1               0.690616        0.353749
  HR1           OH              1               0.690616        0.353749
  HR1           HO              1               0.4005          0
  CN7B          AL              1               0.912425        0.000687836
  CN7B          OS              1               0.849676        0.233255
  CN7B          OH              1               0.849676        0.233255
  CN7B          HO              1               0.63671         0
  HN7           AL              1               0.81383         0.000721408
  HN7           OS              1               0.742799        0.24464
  HN7           OH              1               0.742799        0.24464
  HN7           HO              1               0.484974        0
  CT2           AL              1               0.902563        0.00114065
  CT2           OS              1               0.839077        0.38681
  CT2           OH              1               0.839077        0.38681
  CT2           HO              1               0.622495        0
  CT3           AL              1               0.902563        0.00114065
  CT3           OS              1               0.839077        0.38681
  CT3           OH              1               0.839077        0.38681
  CT3           HO              1               0.622495        0
  NTF2          AL              1               0.867249        0.00200537
  NTF2          OS              1               0.800968        0.680049
  NTF2          OH              1               0.800968        0.680049
  NTF2          HO              1               0.570088        0
  STF2          AL              1               0.884375        0.00243187
  STF2          OS              1               0.819482        0.824681
  STF2          OH              1               0.819482        0.824681
  STF2          HO              1               0.595819        0
  CTF2          AL              1               0.881544        0.00124952
  CTF2          OS              1               0.816425        0.423729
  CTF2          OH              1               0.816425        0.423729
  CTF2          HO              1               0.591608        0
  OTF2          AL              1               0.850365        0.00222884
  OTF2          OS              1               0.782656        0.755833
  OTF2          OH              1               0.782656        0.755833
  OTF2          HO              1               0.544059        0
  FTF2          AL              1               0.849776        0.00111972
  FTF2          OS              1               0.782017        0.379712
  FTF2          OH              1               0.782017        0.379712
  FTF2          HO              1               0.543139        0

[ bondtypes ]
```

```
; C2MIM
; i          j          func       b0 (nm)      kb (kJ/mol/nm2)
  CN7B       NR1        1          0.14762      0.092048E+06
  CPH1       NR1        1          0.13819      0.16736E+06
  CPH2       NR1        1          0.13366      0.16736E+06
  CPH1       CPH1       1          0.1361       0.171544E+06
  CPH2       HR1        1          0.10779      0.142256E+06
  CPH1       HR3        1          0.10775      0.152716E+06
  CN7B       HN7        1          0.10899      0.129286E+06
  CT3        HN7        1          0.10935      0.134725E+06
  CN7B       CT3        1          0.15308      0.08368E+06
; NTF2
; i          j          func       b0 (nm)      kb (kJ/mol/nm2)
  CTF2       FTF2       1          0.1323       0.18485E+06
  CTF2       STF2       1          0.1818       0.0985001E+06
  STF2       OTF2       1          0.1442       0.26655E+06
  NTF2       STF2       1          0.157        0.15565E+06

[ angletypes ]
; C2MIM
; i          j          k          func         th0 (deg)    kth (kJ/mol/rad2)
  CT2        CN7B       NR1        1            112.34       0.58576E+03
  CPH1       NR1        CPH2       1            108.25       0.54392E+03
  HN7        CN7B       NR1        1            109.41       0.12552E+03
  HR1        CPH2       NR1        1            125.44       0.1046E+03
  NR1        CPH1       CPH1       1            107.28       0.54392E+03
  NR1        CPH2       NR1        1            109.11       0.54392E+03
  HR3        CPH1       CPH1       1            130.74       0.1046E+03
  NR1        CPH1       HR3        1            122.04       0.1046E+03
  HN7        CN7B       HN7        1            108.44       0.148532E+03
  HN7        CN7B       CT2        1            111.68       0.139746E+03
  HN7        CT2        CN7B       1            109.13       0.139746E+03
  CN7B       CT2        CT2        1            111.50       0.244136E+03
  CT2        CT2        CT3        1            112.34       0.242672E+03
  HN7        CT2        HN7        1            106.13       0.148532E+03
  HN7        CT3        HN7        1            107.24       0.148532E+03
  CT2        CT2        HN7        1            108.43       0.110876E+03
  CT3        CT2        HN7        1            109.47       0.144766E+03
  CT2        CT3        HN7        1            111.62       0.144766E+03
  CN7B       NR1        CPH2       1            125.75       0.54392E+03
  CN7B       NR1        CPH1       1            125.67       0.54392E+03
  CT3        CN7B       NR1        1            112.34       0.58576E+03
  HN7        CN7B       CT3        1            111.68       0.139746E+03
  HN7        CT3        CN7B       1            109.13       0.139746E+03
  CT2        CT2        CT2        1            114.27       0.244136E+03
; NTF2
; i          j          k          func         th0 (deg)    kth (kJ/mol/rad2)
  FTF2       CTF2       FTF2       1            107.10       0.390493E+03
  STF2       CTF2       FTF2       1            111.80       0.346979E+03
  CTF2       STF2       OTF2       1            102.60       0.43501E+03
  OTF2       STF2       OTF2       1            118.50       0.484507E+03
  OTF2       STF2       NTF2       1            113.60       0.39543E+03
  CTF2       STF2       NTF2       1            100.20       0.407982E+03
  STF2       NTF2       STF2       1            125.60       0.335515E+03

[ dihedraltypes ]
; C2MIM
; i          j          k          l          func         phi0 (deg)   kphi (kJ/mol)  n
  CPH2       NR1        CPH1       CPH1       1            180          58.576         2
  NR1        CPH1       CPH1       NR1        1            180          58.576         2
  NR1        CPH2       NR1        CPH1       1            180          58.576         2
  HR1        CPH2       NR1        CPH1       1            180          12.552         2
  HR3        CPH1       CPH1       HR3        1            180          8.368          2
  CPH1       CPH1       NR1        CN7B       1            0            0              1
  HR3        CPH1       NR1        CPH2       1            180          12.552         2
  NR1        CPH1       CPH1       HR3        1            180          12.552         2
  NR1        CPH2       NR1        CN7B       1            180          0              2
  HR1        CPH2       NR1        CN7B       1            180          0              2
  HR3        CPH1       NR1        CN7B       1            180          0              2
  CPH2       NR1        CN7B       HN7        1            180          0.81588        2
  CPH1       NR1        CN7B       HN7        1            0            0              3
  CPH2       NR1        CN7B       CT2        1            180          0.4184         3
  CPH1       NR1        CN7B       CT2        1            0            0.8368         4
  NR1        CN7B       CT2        CT2        1            0            0              3
  HN7        CT2        CT3        HN7        1            0            0.66944        3
  CT2        CT2        CT3        HN7        1            0            0.66944        3
  NR1        CN7B       CT2        HN7        1            0            0              3
  CN7B       CT2        CT2        CT3        1            0            0.6276         1
  HN7        CN7B       CT2        HN7        1            0            0.81588        3
  HN7        CN7B       CT2        CT2        1            0            0.81588        3
  HN7        CT2        CT2        HN7        1            0            0.81588        3
  CN7B       CT2        CT2        HN7        1            0            0.81588        3
  HN7        CT2        CT2        CT3        1            0            0.81588        3
  CPH2       NR1        CN7B       CT3        1            180          0.4184         3
  CPH1       NR1        CN7B       CT3        1            0            0.8368         4
  NR1        CN7B       CT3        HN7        1            0            0              3
  HN7        CN7B       CT3        HN7        1            0            0.81588        3
  CT2        CT2        CT2        CT2        1            0            0.81588        3
  CT2        CT2        CT2        CT3        1            0            0.81588        3
  CN7B       CT2        CT2        CT2        1            0            0.81588        3
  CT2        CT2        CT2        HN7        1            0            0.81588        3
; C2MIM (impropers)
; i          j          k          l          func         xi0 (deg)    kxi (kJ/mol/rad2)
```

```
  CPH2          NR1           NR1           HR1           2             0             2.09200
  NR1           CPH1          CPH2          CN7B          2             0             2.51040
  CPH1          CPH1          NR1           HR3           2             0             2.09200
; NTF 2
; i             j             k             l             func          phi0 (deg)    kphi (kJ/mol)  n
  FTF2          CTF2          STF2          OTF2          1             0             0.725506       3
  STF2          NTF2          STF2          OTF2          1             0             -0.0075312     3
  FTF2          CTF2          STF2          NTF2          1             0             0.661072       3
  STF2          NTF2          STF2          CTF2          9             0             32.7729        1
  STF2          NTF2          STF2          CTF2          9             180           -10.4198       2
  STF2          NTF2          STF2          CTF2          9             0             -3.1949        3


[ moleculetype ]
; name          nrexcl
  alu           1

[ atoms ]
; nr            type          resnr         residue       name          cgnr          charge
  1             AL            1             alu           al            1             1.57500


[ moleculetype ]
; name          nrexcl
  oxy           1

[ atoms ]
; nr            type          resnr         residue       atom          cgnr          charge
  1             OS            1             oxy           os            1             -1.05000


[ moleculetype ]
; name          nrexcl
  ohy           2

[ atoms ]
; nr            type          resnr         residue       atom          cgnr          charge
  1             OH            1             ohy           oh            1             -0.95000
  2             HO            1             ohy           ho            2             0.42500

[ bonds ]
; i             j             func          b0 (nm)       kb (kJ/mol/nm2)
  2             1             1             0.10000       0.4637001E+06


[ moleculetype ]
; name          nrexcl
  c2            3

[ atoms ]
; nr            type          resnr         residue       name          cgnr          charge
  1             CPH1          1             c2            cw            1             -0.147177
  2             NR1           1             c2            na            2             0.193715
  3             CPH2          1             c2            cr            3             -0.091215
  4             NR1           1             c2            na            4             0.059417
  5             CPH1          1             c2            cw            5             -0.134873
  6             CN7B          1             c2            c1            6             -0.250840
  7             CN7B          1             c2            c1            7             0.103944
  8             CT3           1             c2            ce            8             -0.104555
  9             HN7           1             c2            h1            9             0.145165
  10            HN7           1             c2            h1            10            0.145165
  11            HN7           1             c2            h1            11            0.145165
  12            HN7           1             c2            h1            12            0.055550
  13            HN7           1             c2            h1            13            0.055550
  14            HR3           1             c2            hb            14            0.209995
  15            HR3           1             c2            hb            15            0.220374
  16            HR1           1             c2            ha            16            0.218877
  17            HN7           1             c2            hc            17            0.058581
  18            HN7           1             c2            hc            18            0.058581
  19            HN7           1             c2            hc            19            0.058581

[ bonds ]
; i             j
  6             2
  2             1
  1             5
  5             4
  4             3
  3             2
  4             7
  7             8
```

```
  9             6
  10            6
  11            6
  3             16
  5             15
  1             14
  7             12
  7             13
  8             17
  8             18
  8             19

[ angles ]
; i             j             k
  2             1             5
  2             1             14
  5             1             14
  1             2             3
  1             2             6
  3             2             6
  2             3             4
  2             3             16
  4             3             16
  3             4             5
  3             4             7
  5             4             7
  1             5             4
  1             5             15
  4             5             15
  2             6             9
  2             6             10
  2             6             11
  9             6             10
  9             6             11
  10            6             11
  4             7             8
  4             7             12
  4             7             13
  8             7             12
  8             7             13
  12            7             13
  7             8             17
  7             8             18
  7             8             19
  17            8             18
  17            8             19
  18            8             19

[ dihedrals ]
; i             j             k             l
  9             6             2             1
  9             6             2             3
  10            6             2             1
  10            6             2             3
  11            6             2             1
  11            6             2             3
  6             2             1             5
  6             2             1             14
  3             2             1             5
  3             2             1             14
  2             1             5             4
  2             1             5             15
  14            1             5             4
  14            1             5             15
  1             5             4             3
  1             5             4             7
  15            5             4             3
  15            5             4             7
  5             4             3             2
  5             4             3             16
  7             4             3             2
  7             4             3             16
  4             3             2             6
  4             3             2             1
  16            3             2             6
  16            3             2             1
  5             4             7             12
  5             4             7             13
  5             4             7             8
  3             4             7             12
  3             4             7             13
  3             4             7             8
  4             7             8             17
  4             7             8             18
  4             7             8             19
  12            7             8             17
  12            7             8             18
  12            7             8             19
  13            7             8             17
  13            7             8             18
  13            7             8             19
; impropers
  3             4             2             16            2
```

```
  4             5             3             7             2
  2             1             3             6             2
  1             5             2             14            2
  5             1             4             15            2

[ pairs ]
; i             j
  9             1
  9             3
  10            1
  10            3
  11            1
  11            3
  6             5
  6             14
  3             5
  3             14
  2             4
  2             15
  14            4
  14            15
  1             3
  1             7
  15            3
  15            7
  5             2
  5             16
  7             2
  7             16
  4             6
  4             1
  16            6
  16            1
  5             12
  5             13
  5             8
  3             12
  3             13
  3             8
  4             17
  4             18
  4             19
  12            17
  12            18
  12            19
  13            17
  13            18
  13            19



[ moleculetype ]
; name          nrexcl
  ntf2          3

[ atoms ]
; nr            type          resnr         residue       name          cgnr
  1             CTF2          1             ntf2          c             1
  2             FTF2          1             ntf2          f             2
  3             FTF2          1             ntf2          f             3
  4             STF2          1             ntf2          s             4
  5             OTF2          1             ntf2          o             5
  6             FTF2          1             ntf2          f             6
  7             OTF2          1             ntf2          o             7
  8             NTF2          1             ntf2          n             8
  9             STF2          1             ntf2          s             9
  10            OTF2          1             ntf2          o             10
  11            OTF2          1             ntf2          o             11
  12            CTF2          1             ntf2          c             12
  13            FTF2          1             ntf2          f             13
  14            FTF2          1             ntf2          f             14
  15            FTF2          1             ntf2          f             15

[ bonds ]
; i             j
  1             2
  1             3
  1             6
  1             4
  4             5
  4             7
  4             8
  8             9
  9             10
  9             11
  9             12
  12            13
  12            14
  12            15

[ angles ]
```

```
; i            j            k
  2            1            3
  2            1            4
  2            1            6
  3            1            4
  3            1            6
  4            1            6
  1            4            5
  1            4            7
  1            4            8
  5            4            7
  5            4            8
  7            4            8
  4            8            9
  8            9            10
  8            9            11
  8            9            12
  10           9            11
  10           9            12
  11           9            12
  9            12           13
  9            12           14
  9            12           15
  13           12           14
  13           12           15
  14           12           15

[ dihedrals ]
; i            j            k            l
; x            C            S            x
  2            1            4            8
  2            1            4            5
  2            1            4            7
  3            1            4            8
  3            1            4            5
  3            1            4            7
  6            1            4            8
  6            1            4            5
  6            1            4            7
  13           12           9            8
  14           12           9            8
  15           12           9            8
  13           12           9            10
  13           12           9            11
  14           12           9            10
  14           12           9            11
  15           12           9            10
; x            N            S            x
  4            8            9            12
  4            8            9            10
  4            8            9            11
  9            8            4            1
  9            8            4            5
  9            8            4            7

[ pairs ]
; i            j
  2            8
  2            5
  2            7
  3            8
  3            5
  3            7
  6            8
  6            5
  6            7
  13           8
  14           8
  15           8
  13           10
  13           11
  14           10
  14           11
  15           10
  4            12
  4            10
  4            11
  9            1
  9            5
  9            7


[ system ]
; name
  C2MIM-NTF2 according to Maginn et al.

[ molecules ]
; name         number
  c2           1686
  ntf2         1686
  alu          4845
  oxy          6885
  ohy          765
```

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