Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Information

A Theoretical study on lidocaine solubility in deep eutectic solvents

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Table S1 Force field parameterization used for MD simulations

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The general form of the applied force field is:

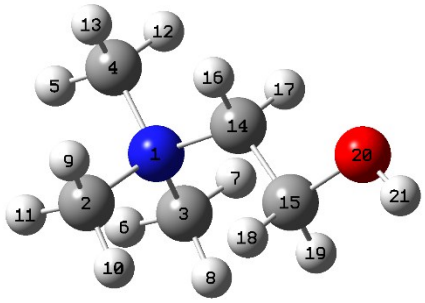
$$E = \sum_{bonds} k_r (r - r_{eq})^2 + \sum_{angles} k_\theta (\theta - \theta_{eq})^2 + E_{tor}$$

$$+ \sum_i \sum_j \left\{ 4\varepsilon_{ij} \left[\left(\frac{\sigma_{ij}}{r_{ij}} \right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}} \right)^{6} \right] + \frac{q_i q_j e^2}{4\pi\varepsilon_0 r_{ij}} \right\}$$

Graphene was maintained as rigid along the simulations, thus dihedrals (E_{tor}) were null for all the molecules.

Improper dihedrals were described according to:

$$E_{improper} = k_\phi(\phi - \phi_0)^2$$



Ch

Atoms

q	σ_{ii} / Å	ε_{ii}/ kJ mol^{-1}	#
0.27770	3.1000	0.8370	1
-0.40920	3.4500	0.3350	2
-0.41500	3.4500	0.3350	3
-0.54830	3.4500	0.3350	4
0.21190	2.2100	0.0920	5
0.18860	2.2100	0.0920	6
0.16780	2.2100	0.0920	7
0.19770	2.2100	0.0920	8
0.18540	2.2100	0.0920	9
0.23740	2.2100	0.0920	10
0.16670	2.2100	0.0920	11
0.21050	2.2100	0.0920	12
0.20910	2.2100	0.0920	13
-0.36350	3.6400	0.2300	14
0.37580	3.6400	0.2300	15
0.19220	2.2100	0.0920	16
0.14290	2.2100	0.0920	17
-0.00030	2.2100	0.0920	18
0.03390	2.2100	0.0920	19
-0.65920	3.1538	0.6370	20
0.40360	0.4000	0.1925	21

Bonds

Atom Numbers		r_{eq} /Å	k_r/ kJ mol^{-1} Å^{-2}
1	2	1.5100	1092.80
1	3	1.5100	1092.80
1	14	1.5320	1092.80
1	4	1.5100	1092.80
2	9	1.0890	1422.56
2	10	1.0890	1422.56
2	11	1.0890	1422.56
3	6	1.0890	1422.56
3	7	1.0890	1422.56
3	8	1.0890	1422.56
4	5	1.0890	1422.56
4	12	1.0890	1422.56
4	13	1.0890	1422.56
14	15	1.5200	931.60
14	16	1.0910	1422.56
14	17	1.0910	1422.56
15	18	1.0960	1422.56
15	19	1.0960	1422.56
15	20	1.4180	1792.00
20	21	0.9650	2313.80

Angles

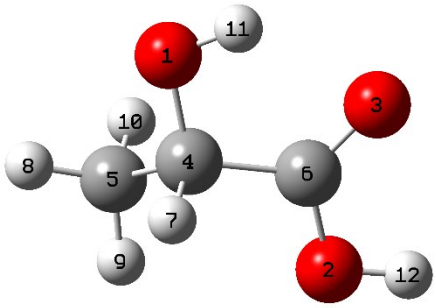
Atom Numbers			θ_{eq} / deg	k_θ / kJ mol^{-1} rad^{-2}
2	1	3	108.9000	209.30
2	1	14	110.7000	209.30
2	1	4	108.9000	209.30
3	1	14	110.7000	209.30
3	1	4	108.9000	209.30
14	1	4	110.7000	209.30
1	2	10	109.0000	201.00
1	2	11	109.0000	201.00
1	2	9	109.0000	201.00
10	2	11	109.3000	148.60
10	2	9	109.3000	148.60
11	2	9	109.3000	148.60
1	3	8	109.0000	201.00
1	3	7	109.0000	201.00
1	3	6	109.0000	201.00
8	3	7	109.3000	148.60
8	3	6	109.3000	148.60
7	3	6	109.3000	148.60
1	4	13	109.0000	201.00
1	4	12	109.0000	201.00
1	4	5	109.0000	201.00
13	4	12	109.3000	148.60
13	4	5	109.3000	148.60
12	4	5	109.3000	148.60
1	14	15	110.6000	334.90
1	14	16	106.2000	215.60
1	14	17	106.2000	215.60
15	14	16	110.6000	110.90
15	14	17	110.6000	110.90
16	14	17	108.4000	148.60

14	15	18	105.8000	148.60	
14	15	19	105.8000	148.60	
14	15	20	109.4000	316.90	
18	15	19	107.2000	148.60	
18	15	20	111.8000	192.20	
19	15	20	111.8000	192.20	
15	20	21	111.9000	240.70	

Dihedrals

Atom Numbers				**δ / deg**	**k_Φ / kJ mol^{-1}**	**m**
3	1	2	10	0.00	0.335	3
3	1	2	11	0.00	0.335	3
3	1	2	9	0.00	0.335	3
14	1	2	10	0.00	0.335	3
14	1	2	11	0.00	0.335	3
14	1	2	9	0.00	0.335	3
4	1	2	10	0.00	0.335	3
4	1	2	11	0.00	0.335	3
4	1	2	9	0.00	0.335	3
2	1	3	8	0.00	0.335	3
2	1	3	7	0.00	0.335	3
2	1	3	6	0.00	0.335	3
14	1	3	8	0.00	0.335	3
14	1	3	7	0.00	0.335	3
14	1	3	6	0.00	0.335	3
4	1	3	8	0.00	0.335	3
4	1	3	7	0.00	0.335	3
4	1	3	6	0.00	0.335	3
2	1	14	15	180.00	10.500	3
2	1	14	16	0.00	0.335	3
2	1	14	17	0.00	0.335	3
3	1	14	15	180.00	10.500	3
3	1	14	16	0.00	0.335	3
3	1	14	17	0.00	0.335	3
4	1	14	15	180.00	10.500	3
4	1	14	16	0.00	0.335	3
4	1	14	17	0.00	0.335	3
2	1	4	13	0.00	0.335	3
2	1	4	12	0.00	0.335	3
2	1	4	5	0.00	0.335	3
3	1	4	13	0.00	0.335	3
3	1	4	12	0.00	0.335	3
3	1	4	5	0.00	0.335	3
14	1	4	13	0.00	0.335	3
14	1	4	12	0.00	0.335	3
14	1	4	5	0.00	0.335	3
1	14	15	18	0.00	2.510	2
1	14	15	19	0.00	2.510	2
1	14	15	20	0.00	0.000	1
16	14	15	18	180.00	10.500	2
16	14	15	19	180.00	10.500	2
16	14	15	20	180.00	0.000	2
17	14	15	18	180.00	10.500	2
17	14	15	19	180.00	10.500	2
17	14	15	20	180.00	0.000	2

14	15	20	21	0.00	5.440	1
18	15	20	21	0.00	1.260	2
19	15	20	21	0.00	1.260	2



LA in ChCl:LA 1:1

Atoms

q	σ_{ii} / Å	ε_{ii}/ kJ mol^{-1}	#
-0.64260	3.15378	0.636386	2
-0.57590	3.02905	0.502080	3
0.52070	3.87541	0.230120	4
-0.48520	3.87541	0.230120	5
0.55010	3.56359	0.460240	6
-0.00620	2.35197	0.092048	7
0.13920	2.35197	0.092048	8
0.12520	2.35197	0.092048	9
0.13560	2.35197	0.092048	10
0.34980	0.40001	0.192464	11
0.47630	0.40001	0.192464	12

Bonds

Atom Numbers		r_{eq} /Å	k_r/ kJ mol^{-1} Å^{-2}
1	4	1.418	1519.6875
1	11	0.972	2346.8265
2	6	1.355	1746.7195
2	12	0.981	2229.093
3	6	1.222	3899.333
4	5	1.508	1282.1115
4	6	1.492	1261.639
4	7	1.093	1435.0745
5	8	1.093	1435.0745
5	9	1.093	1435.0745
5	10	1.093	1435.0745

Angles

Atom Numbers			θ_{eq} / deg	k_θ / kJ mol^{-1} rad^{-2}
4	1	11	106.503	477.55
6	2	12	111.948	351.09
1	4	5	108.133	597.39
1	4	6	104.112	317.97
1	4	7	108.577	470.32
5	4	6	107.517	467.91
5	4	7	110.549	383

6	4	7	108.385	391.44
4	5	8	110.549	383
4	5	9	110.549	383
4	5	10	110.549	383
8	5	9	108.836	310.74
8	5	10	108.836	310.74
9	5	10	108.836	310.74
2	6	3	124.425	695.55
2	6	4	109.716	628.1
3	6	4	124.41	564.87

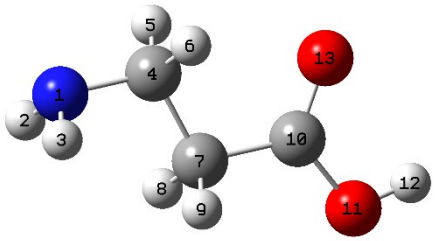
Dihedrals

Atom Numbers				**δ / deg**	**k_ϕ / kJ mol^{-1}**	**m**
1	4	5	8	0	-1.3682	1
1	4	5	8	180	2.2426	2
1	4	5	8	0	0.5858	3
1	4	5	9	0	-1.3682	1
1	4	5	9	180	2.2426	2
1	4	5	9	0	0.5858	3
1	4	5	10	0	-1.3682	1
1	4	5	10	180	2.2426	2
1	4	5	10	0	0.5858	3
1	4	6	2	0	0.9372	1
1	4	6	2	180	1.364	2
1	4	6	2	0	0.6653	3
1	4	6	3	0	-0.8284	1
1	4	6	3	180	1.5272	2
1	4	6	3	0	-0.2929	3
2	6	4	5	0	-0.2469	1
2	6	4	5	180	-0.6987	2
2	6	4	5	0	0.4226	3
2	6	4	7	180	-1.3054	2
2	6	4	7	0	0.6904	3
3	6	2	12	0	3.4769	1
3	6	2	12	180	12.87	2
3	6	2	12	0	-0.1213	3
3	6	4	5	0	1.7238	1
3	6	4	5	180	0.2929	2
3	6	4	5	0	0.682	3
3	6	4	7	0	1.3807	1
3	6	4	7	180	-2.9455	2
3	6	4	7	0	0.6443	3
4	6	2	12	0	-2.4393	1
4	6	2	12	180	10.6232	2
4	6	2	12	0	-1.1422	3
5	4	1	11	180	0.5648	2
5	4	1	11	0	0.4937	3
6	4	1	11	0	-3.456	1
6	4	1	11	180	-3.4727	2
6	4	1	11	0	0.5899	3
6	4	5	8	0	-0.5356	1
6	4	5	8	180	0.1213	2
6	4	5	9	0	-0.5356	1
6	4	5	9	180	0.1213	2
6	4	5	10	0	-0.5356	1

6	4	5	10	180	0.1213	2
7	4	1	11	0	1.2468	1
7	4	1	11	180	-0.5774	2
7	4	1	11	0	0.7238	3
7	4	5	8	0	0.5941	1
7	4	5	8	180	-2.8995	2
7	4	5	8	0	0.6569	3
7	4	5	9	0	0.5941	1
7	4	5	9	180	-2.8995	2
7	4	5	9	0	0.6569	3
7	4	5	10	0	0.5941	1
7	4	5	10	180	-2.8995	2
7	4	5	10	0	0.6569	3

Improper

Atom Numbers				φ_0 / deg	k_ϕ / kJ mol^{-1} rad^{-2}
4	6	1	5	0	0
4	5	1	7	0	0
6	2	4	3	0	84.9101
5	8	4	9	0	0
5	8	4	10	0	0



AL

Atoms

q	σ_{ii} / Å	ε_{ii}/ kJ mol^{-1}	#
-1.07224	3.10000	0.837000	1
0.37515	0.40001	0.192464	2
0.37595	0.40001	0.192464	3
0.51712	3.64000	0.230000	4
0.00245	2.21000	0.092000	5
0.01155	2.21000	0.092000	6
-0.41578	3.64000	0.230000	7
0.11232	2.21000	0.092000	8
0.10783	2.21000	0.092000	9
0.91316	3.64000	0.230000	10
-0.69057	3.15378	0.636386	11
0.52387	0.40001	0.192464	12
-0.79452	3.02905	0.502080	13

Bonds

Atom Numbers		r_{eq} /Å	k_r/ kJ mol^{-1} Å^{-2}
1	2	1.019	1954.183
1	3	1.019	1954.183

1	4	1.451	1530.825
4	5	1.093	1435.0745
4	6	1.093	1435.0745
4	7	1.508	1282.1115
7	8	1.093	1435.0745
7	9	1.093	1435.0745
7	10	1.492	1261.639
10	11	1.355	1746.7195
10	13	1.222	3899.333
11	12	0.981	2229.093

Angles

Atom Numbers			**θ_{eq} / deg**	**k_θ / kJ mol^{-1} rad^{-2}**
2	1	3	105.998	358.32
2	1	4	109.062	459.49
3	1	4	109.062	459.49
1	4	5	110.297	393.25
1	4	6	110.297	393.25
1	4	7	108.290	467.91
5	4	6	108.836	310.74
5	4	7	110.549	383
6	4	7	110.549	383
4	7	8	110.549	383
4	7	9	110.549	383
4	7	10	107.517	467.91
8	7	9	108.836	310.74
8	7	10	108.385	391.44
9	7	10	108.385	391.44
7	10	11	109.716	628.1
7	10	13	124.410	564.87
11	10	13	124.425	695.55
10	11	12	111.948	351.09

Dihedrals

Atom Numbers				**δ / deg**	**k_ϕ / kJ mol^{-1}**	**m**
1	4	7	8	0	-1.5564	1
1	4	7	8	180	-2.5815	2
1	4	7	8	0	0.7071	3
1	4	7	9	0	-1.5564	1
1	4	7	9	180	-2.5815	2
1	4	7	9	0	0.7071	3
1	4	7	10	0	0.6276	3
2	1	4	5	0	-0.318	1
2	1	4	5	180	-0.9205	2
2	1	4	5	0	0.7448	3
2	1	4	6	0	-0.318	1
2	1	4	6	180	-0.9205	2
2	1	4	6	0	0.7448	3
2	1	4	7	0	-0.8954	1
2	1	4	7	180	0.6778	2
2	1	4	7	0	0.5858	3
3	1	4	5	0	-0.318	1
3	1	4	5	180	-0.9205	2
3	1	4	5	0	0.7448	3
3	1	4	6	0	-0.318	1

3	1	4	6	180	-0.9205	2
3	1	4	6	0	0.7448	3
3	1	4	7	0	-0.8954	1
3	1	4	7	180	0.6778	2
3	1	4	7	0	0.5858	3
4	7	10	11	0	-0.2469	1
4	7	10	11	180	-0.6987	2
4	7	10	11	0	0.4226	3
4	7	10	13	0	1.7238	1
4	7	10	13	180	0.2929	2
4	7	10	13	0	0.682	3
5	4	7	8	0	0.5941	1
5	4	7	8	180	-2.8995	2
5	4	7	8	0	0.6569	3
5	4	7	9	0	0.5941	1
5	4	7	9	180	-2.8995	2
5	4	7	9	0	0.6569	3
5	4	7	10	0	-0.5356	1
5	4	7	10	180	0.1213	2
6	4	7	8	0	0.5941	1
6	4	7	8	180	-2.8995	2
6	4	7	8	0	0.6569	3
6	4	7	9	0	0.5941	1
6	4	7	9	180	-2.8995	2
6	4	7	9	0	0.6569	3
6	4	7	10	0	-0.5356	1
6	4	7	10	180	0.1213	2
7	10	11	12	0	-2.4393	1
7	10	11	12	180	10.6232	2
7	10	11	12	0	-1.1422	3
8	7	10	11	180	-1.3054	2
8	7	10	11	0	0.6904	3
8	7	10	13	0	1.3807	1
8	7	10	13	180	-2.9455	2
8	7	10	13	0	0.6443	3
9	7	10	11	180	-1.3054	2
9	7	10	11	0	0.6904	3
9	7	10	13	0	1.3807	1
9	7	10	13	180	-2.9455	2
9	7	10	13	0	0.6443	3
12	11	10	13	0	3.4769	1
12	11	10	13	180	12.87	2
12	11	10	13	0	-0.1213	3

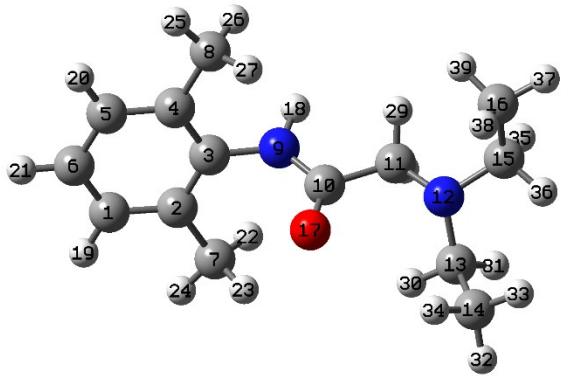
Improper

Atom Numbers				**φ_0 / deg**	**k_ϕ / kJ mol^{-1} rad^{-2}**
1	2	4	3	0	0
4	7	1	5	0	0
4	5	1	6	0	0
7	10	4	8	0	0
7	8	4	9	0	0
10	11	7	13	0	84.9101

LA in AL:LA 1:1

q	#
-0.74485	1
-0.68487	2
-0.60333	3
0.64553	4
-0.44528	5
0.48799	6
-0.03279	7
0.13211	8
0.10608	9
0.11828	10
0.41101	11
0.64384	12

The remaining force field parameters as for LA in ChCl:LA 1:1



LD

Atoms

q	σ_{ii} / Å	ε_{ii}/ kJ mol^{-1}	#
-0.1200	3.5490	0.2930	1
-0.0400	3.5490	0.2930	2
0.1800	3.5490	0.2930	3
-0.0400	3.5490	0.2930	4
-0.1200	3.5490	0.2930	5
-0.0600	3.5490	0.2930	6
-0.2000	3.6705	0.3350	7
-0.2000	3.6705	0.3350	8
-0.6100	3.2963	0.8374	9
0.4800	3.5636	0.4606	10
-0.0100	3.8754	0.2302	11
-0.4800	3.2970	0.8374	12
-0.0400	3.8754	0.2302	13
-0.2500	3.6705	0.3350	14
-0.0400	3.8754	0.2302	15
-0.2500	3.6705	0.3350	16
-0.4800	3.0290	0.5024	17

0.2400	0.4000	0.1926	18
0.1000	2.4200	0.1260	19
0.1000	2.4200	0.1260	20
0.1000	2.4200	0.1260	21
0.1000	2.3520	0.0921	22
0.1000	2.3520	0.0921	23
0.1000	2.3520	0.0921	24
0.1000	2.3520	0.0921	25
0.1000	2.3520	0.0921	26
0.1000	2.3520	0.0921	27
0.1000	2.3520	0.0921	28
0.1000	2.3520	0.0921	29
0.1000	2.3520	0.0921	30
0.1000	2.3520	0.0921	31
0.0900	2.3520	0.0921	32
0.0900	2.3520	0.0921	33
0.0900	2.3520	0.0921	34
0.1000	2.3520	0.0921	35
0.1000	2.3520	0.0921	36
0.0900	2.3520	0.0921	37
0.0900	2.3520	0.0921	38
0.0900	2.3520	0.0921	39

Bonds

Atom Numbers		**r_{eq} /Å**	**k_r/ kJ mol^{-1} Å^{-2}**
1	2	1.37500	1277.00
1	6	1.37500	1277.00
1	19	1.08000	1423.00
2	3	1.37500	1277.00
2	7	1.49000	963.00
3	4	1.37500	1277.00
3	9	1.36600	1507.00
4	5	1.37500	1277.00
4	8	1.49000	963.00
5	6	1.37500	1277.00
5	20	1.08000	1423.00
6	21	1.08000	1423.00
7	22	1.11100	1348.00
7	23	1.11100	1348.00
7	24	1.11100	1348.00
8	25	1.11100	1348.00
8	26	1.11100	1348.00
8	27	1.11100	1348.00
9	10	1.34500	1549.00
9	18	0.98000	1696.00
10	11	1.49000	1047.00
10	17	1.23000	2596.00
11	12	1.43000	1340.00
11	28	1.11100	1294.00
11	29	1.11100	1294.00
12	13	1.43000	1340.00
12	15	1.43000	1340.00
13	14	1.52800	944.00
13	30	1.11100	1294.00
13	31	1.11100	1294.00

14	32	1.11100	1348.00
14	33	1.11100	1348.00
14	34	1.11100	1348.00
15	16	1.52800	944.00
15	35	1.11100	1294.00
15	36	1.11100	1294.00
16	37	1.11100	1348.00
16	38	1.11100	1348.00
16	39	1.11100	1348.00

Angles

Atom Numbers			θ_{eq} / deg	k_θ / kJ mol^{-1} rad^{-2}
2	1	6	120	167.5
2	1	19	120	125.6
6	1	19	120	125.6
1	2	3	120	167.5
1	2	7	122.3	191.8
3	2	7	122.3	191.8
2	3	4	120	167.5
2	3	9	119.5	209
4	3	9	119.5	209
3	4	5	120	167.5
3	4	8	122.3	191.8
5	4	8	122.3	191.8
4	5	6	120	167.5
4	5	20	120	125.6
6	5	20	120	125.6
1	6	5	120	167.5
1	6	21	120	125.6
5	6	21	120	125.6
2	7	22	107.5	206.4
2	7	23	107.5	206.4
2	7	24	107.5	206.4
22	7	23	108.4	148.6
22	7	24	108.4	148.6
23	7	24	108.4	148.6
4	8	25	107.5	206.4
4	8	26	107.5	206.4
4	8	27	107.5	206.4
25	8	26	108.4	148.6
25	8	27	108.4	148.6
26	8	27	108.4	148.6
3	9	10	120	209.35
3	9	18	111	209.3
10	9	18	111	209.3
9	10	11	116.5	335
9	10	17	122.5	335
11	10	17	121	335
10	11	12	107	209.4
10	11	28	109.5	138.1
10	11	29	109.5	138.1
12	11	28	109.5	215.6
12	11	29	109.5	215.6
28	11	29	109	148.6
11	12	13	111	418.7

11	12	15	111	418.7
13	12	15	111	418.7
12	13	14	113.5	293.1
12	13	30	109.5	215.6
12	13	31	109.5	215.6
14	13	30	110.1	144.9
14	13	31	110.1	144.9
30	13	31	109	148.6
13	14	32	110.1	144.9
13	14	33	110.1	144.9
13	14	34	110.1	144.9
32	14	33	108.4	148.6
32	14	34	108.4	148.6
33	14	34	108.4	148.6
12	15	16	113.5	293.1
12	15	35	109.5	215.6
12	15	36	109.5	215.6
16	15	35	110.1	144.9
16	15	36	110.1	144.9
35	15	36	109	148.6
15	16	37	110.1	144.9
15	16	38	110.1	144.9
15	16	39	110.1	144.9
37	16	38	108.4	148.6
37	16	39	108.4	148.6
38	16	39	108.4	148.6

Dihedrals

	Atom Numbers			**δ / deg**	**k_ϕ / kJ mol^{-1}**	**m**
6	1	2	3	180	13	2
6	1	2	7	180	13	2
19	1	2	3	180	17.6	2
19	1	2	7	180	17.6	2
2	1	6	5	180	13	2
2	1	6	21	180	17.6	2
19	1	6	5	180	17.6	2
19	1	6	21	180	10	2
1	2	3	4	180	13	2
1	2	3	9	180	13	2
7	2	3	4	180	13	2
7	2	3	9	180	13	2
1	2	7	22	0	0	0
1	2	7	23	0	0	0
1	2	7	24	0	0	0
3	2	7	22	0	0	0
3	2	7	23	0	0	0
3	2	7	24	0	0	0
2	3	4	5	180	13	2
2	3	4	8	180	13	2
9	3	4	5	180	13	2
9	3	4	8	180	13	2
2	3	9	10	0	3.3	3
2	3	9	18	180	4.2	2
4	3	9	10	0	3.3	3
4	3	9	18	180	4.2	2

3	4	5	6	180	13	2
3	4	5	20	180	17.6	2
8	4	5	6	180	13	2
8	4	5	20	180	17.6	2
3	4	8	25	0	0	0
3	4	8	26	0	0	0
3	4	8	27	0	0	0
5	4	8	25	0	0	0
5	4	8	26	0	0	0
5	4	8	27	0	0	0
4	5	6	1	180	13	2
4	5	6	21	180	17.6	2
20	5	6	1	180	17.6	2
20	5	6	21	180	10	2
3	9	10	11	0	6.7	1
3	9	10	11	180	10.47	2
3	9	10	17	180	10.46	2
18	9	10	11	180	10.46	2
18	9	10	17	180	10.46	2
9	10	11	12	0	2.5	1
9	10	11	28	0	0	1
9	10	11	29	0	0	1
17	10	11	12	0	0	1
17	10	11	28	0	0	1
17	10	11	29	0	0	1
10	11	12	13	0	3.35	3
10	11	12	15	0	3.35	3
28	11	12	13	0	0	1
28	11	12	15	0	0	1
29	11	12	13	0	0	1
29	11	12	15	0	0	1
11	12	13	14	0	3.35	3
11	12	13	30	0	0	1
11	12	13	31	0	0	1
15	12	13	14	0	3.35	3
15	12	13	30	0	0	1
15	12	13	31	0	0	1
11	12	15	16	0	3.35	3
11	12	15	35	0	0	1
11	12	15	36	0	0	1
13	12	15	16	0	3.35	3
13	12	15	35	0	0	1
13	12	15	36	0	0	1
12	13	14	32	0	0.67	3
12	13	14	33	0	0.67	3
12	13	14	34	0	0.67	3
30	13	14	32	0	0.67	3
30	13	14	33	0	0.67	3
30	13	14	34	0	0.67	3
31	13	14	32	0	0.67	3
31	13	14	33	0	0.67	3
31	13	14	34	0	0.67	3
12	15	16	37	0	0.67	3
12	15	16	38	0	0.67	3
12	15	16	39	0	0.67	3

35	15	16	37	0	0.67	3
35	15	16	38	0	0.67	3
35	15	16	39	0	0.67	3
36	15	16	37	0	0.67	3
36	15	16	38	0	0.67	3
36	15	16	39	0	0.67	3

Table S2 Systems used for MD simulations. *N* stands for the number of the corresponding molecules

$N_{\text{ChCl:LA 1:1 or AL:LA 1:1}}$	N_{LD}	T / K	P / bar
500	0	298	1
500	1	298	1
500	5	298	1
500	10	298	1
500	31	298	1
500	53	298	1
500	111	298	1