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

Electronic Supplementary information

Design of Arginine Based Therapeutic Deep Eutectic Solvents as Drug Solubilization Vehicle for Active Pharmaceutical Ingredient

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Table S1. Forcefield parameterizations for alcohols studied in this work.

The general form of the applied force field is:

$$E = \sum_{bonds} k_r (r - r_{eq})^2 + \sum_{angles} k_\theta (\theta - \theta_{eq})^2 + E_{tor}$$
$$+ \sum_i \sum_j \left\{ 4\varepsilon_{ij} \left[\left(\frac{\sigma_{ij}}{r_{ij}} \right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}} \right)^{6} \right] + \frac{q_i q_j e^2}{4\pi\varepsilon_0 r_{ij}} \right\}$$

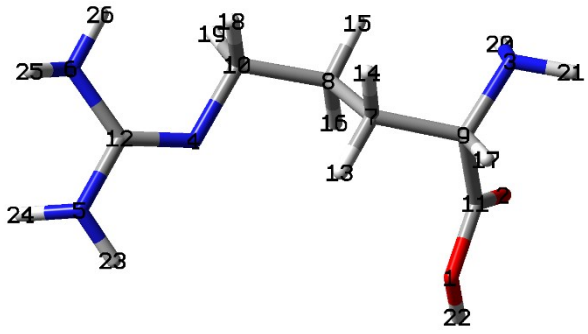
Dihedrals (E_{tor}) were described according to:

$$E_{tor} = \sum_{torsions} k_\phi (1 + \cos(m\phi - \delta))$$

Improper dihedrals were described according to:

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

Lidocaine was described according to the forcefield reported in a previous work (Ref.1)



[Ar]

label	*q*	σ_{ii} / Å	ε_{ii} / kJ mol^{-1}	#
O1	-0.681119	3.15378	0.63639	1
O2	-0.588597	3.02905	0.50208	2
N1	-0.976485	3.29632	0.83680	3
N2	-0.769194	3.29632	0.83680	4
N3	-0.970999	3.29632	0.83680	5
N4	-0.953414	3.29632	0.83680	6
C1	-0.029815	3.87541	0.23012	7
C2	-0.160222	3.87541	0.23012	8
C3	0.260126	3.87541	0.23012	9
C4	0.338029	3.87541	0.23012	10
C5	0.678929	3.56359	0.46024	11

C6	0.919879	3.56359	0.46024	12
H1	0.045548	2.35197	0.09205	13
H2	0.046256	2.35197	0.09205	14
H3	0.029721	2.35197	0.09205	15
H4	0.084089	2.35197	0.09205	16
H5	0.054769	2.35197	0.09205	17
H6	-0.035731	2.35197	0.09205	18
H7	-0.011577	2.35197	0.09205	19
H8	0.368406	0.40001	0.19247	20
H9	0.359452	0.40001	0.19247	21
H10	0.461974	0.40001	0.19247	22
H11	0.38398	0.40001	0.19247	23
H12	0.384711	0.40001	0.19247	24
H13	0.396854	0.40001	0.19247	25
H14	0.364431	0.40001	0.19247	26

Bonds

Atom Numbers		**r_{eq} /Å**	**k_r/ kJ mol^{-1} Å^{-2}**
1	11	1.355	1746.720
1	22	0.981	2229.093
2	11	1.222	3899.333
3	9	1.451	1530.825
3	20	1.019	1954.183
3	21	1.019	1954.183
4	12	1.290	3034.254
4	10	1.458	1434.171
5	12	1.370	1839.764
5	23	1.018	1980.078
5	24	1.018	1980.078
6	12	1.370	1839.764
6	25	1.018	1980.078
6	26	1.018	1980.078
7	9	1.508	1282.112
7	13	1.093	1435.075
7	8	1.508	1282.112
7	14	1.093	1435.075
8	16	1.093	1435.075
8	10	1.508	1282.110
8	15	1.093	1435.075
9	11	1.492	1261.639
9	17	1.093	1435.075
10	18	1.093	1435.075
10	19	1.093	1435.075

Angles

Atom Numbers			**θ_{eq} / deg**	**k_θ / kJ mol^{-1} rad^{-2}**
11	1	22	111.948	351.09
9	3	20	109.062	459.49
9	3	21	109.062	459.49
20	3	21	105.998	358.32
10	4	12	106.409	528.74
12	5	23	114.808	421.55
12	5	24	114.808	421.55
23	5	24	109.16	337.24
12	6	25	114.808	421.55

12	6	26	114.808	421.55
25	6	26	109.16	337.24
8	7	9	109.608	512.48
8	7	13	110.549	383.00
8	7	14	110.549	383.00
9	7	13	110.549	383.00
9	7	14	110.549	383.00
13	7	14	108.836	310.74
7	8	10	109.608	512.48
7	8	15	110.549	383.00
7	8	16	110.549	383.00
10	8	15	110.549	383.00
10	8	16	110.549	383.00
15	8	16	108.836	310.74
3	9	7	108.29	467.91
3	9	11	105.837	720.84
3	9	17	110.297	393.25
7	9	11	107.517	467.91
7	9	17	110.549	383.00
11	9	17	108.385	391.44
4	10	8	108.194	684.11
4	10	18	109.894	441.42
4	10	19	109.894	441.42
8	10	18	110.549	383.00
8	10	19	110.549	383.00
18	10	19	108.836	310.74
1	11	2	124.425	695.55
1	11	9	109.716	628.10
2	11	9	124.41	564.87
4	12	5	128.078	508.26
4	12	6	128.078	508.26
5	12	6	117.002	690.13

Dihedrals

Atom Numbers				**δ / deg**	**k_ϕ / kJ mol^{-1}**	**m**
1	11	9	3	180	0.8368	2
1	11	9	3	0	0.6276	3
1	11	9	7	0	-0.2469	1
1	11	9	7	180	-0.6987	2
1	11	9	7	0	0.4226	3
1	11	9	17	180	-1.3054	2
1	11	9	17	0	0.6904	3
2	11	1	22	0	3.4769	1
2	11	1	22	180	12.87	2
2	11	1	22	0	-0.1213	3
2	11	9	3	180	0.8368	2
2	11	9	3	0	0.8368	3
2	11	9	7	0	1.7238	1
2	11	9	7	180	0.2929	2
2	11	9	7	0	0.682	3
2	11	9	17	0	1.3807	1
2	11	9	17	180	-2.9455	2
2	11	9	17	0	0.6443	3
3	9	7	8	0	-2.9706	1
3	9	7	8	180	-0.1925	2

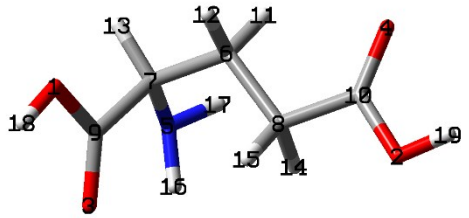
3	9	7	8	0	2.3012	3
3	9	7	13	0	-1.5564	1
3	9	7	13	180	-2.5815	2
3	9	7	13	0	0.7071	3
3	9	7	14	0	-1.5564	1
3	9	7	14	180	-2.5815	2
3	9	7	14	0	0.7071	3
4	10	8	7	0	0.6276	3
4	10	8	15	0	0.6276	3
4	10	8	16	0	0.6276	3
4	12	5	23	0	3.1296	1
4	12	5	23	180	9.1379	2
4	12	5	23	0	-0.8703	3
4	12	5	24	0	3.1296	1
4	12	5	24	180	9.1379	2
4	12	5	24	0	-0.8703	3
4	12	6	25	0	3.1296	1
4	12	6	25	180	9.1379	2
4	12	6	25	0	-0.8703	3
4	12	6	26	0	3.1296	1
4	12	6	26	180	9.1379	2
4	12	6	26	0	-0.8703	3
5	12	4	10	0	-1.5857	1
5	12	4	10	180	38.1079	2
5	12	4	10	0	-0.3933	3
5	12	6	25	0	0.3724	1
5	12	6	25	180	6.5898	2
5	12	6	25	0	1.6276	3
5	12	6	26	0	0.3724	1
5	12	6	26	180	6.5898	2
5	12	6	26	0	1.6276	3
6	12	4	10	0	-1.5857	1
6	12	4	10	180	38.1079	2
6	12	4	10	0	-0.3933	3
6	12	5	23	0	0.3724	1
6	12	5	23	180	6.5898	2
6	12	5	23	0	1.6276	3
6	12	5	24	0	0.3724	1
6	12	5	24	180	6.5898	2
6	12	5	24	0	1.6276	3
7	8	10	18	0	1.3389	1
7	8	10	18	180	-1.318	2
7	8	10	18	0	0.5523	3
7	8	10	19	0	1.3389	1
7	8	10	19	180	-1.318	2
7	8	10	19	0	0.5523	3
7	9	3	20	0	-0.8954	1
7	9	3	20	180	0.6778	2
7	9	3	20	0	0.5858	3
7	9	3	21	0	-0.8954	1
7	9	3	21	180	0.6778	2
7	9	3	21	0	0.5858	3
8	7	9	11	0	0.1381	1
8	7	9	11	180	-0.3264	2
8	7	9	11	0	0.2971	3

8	7	9	17	0	1.3389	1
8	7	9	17	180	-1.318	2
8	7	9	17	0	0.5523	3
9	7	8	10	0	0.2134	1
9	7	8	10	180	1.4267	2
9	7	8	10	0	0.6945	3
9	7	8	15	0	1.3389	1
9	7	8	15	180	-1.318	2
9	7	8	15	0	0.5523	3
9	7	8	16	0	1.3389	1
9	7	8	16	180	-1.318	2
9	7	8	16	0	0.5523	3
9	11	1	22	0	-2.4393	1
9	11	1	22	180	10.6232	2
9	11	1	22	0	-1.1422	3
10	8	7	13	0	1.3389	1
10	8	7	13	180	-1.318	2
10	8	7	13	0	0.5523	3
10	8	7	14	0	1.3389	1
10	8	7	14	180	-1.318	2
10	8	7	14	0	0.5523	3
11	9	3	20	180	-0.6276	2
11	9	3	20	0	1.046	3
11	9	3	21	180	-0.6276	2
11	9	3	21	0	1.046	3
11	9	7	13	0	-0.5356	1
11	9	7	13	180	0.1213	2
11	9	7	14	0	-0.5356	1
11	9	7	14	180	0.1213	2
12	4	10	18	0	0.4268	1
12	4	10	18	180	-0.7029	2
12	4	10	18	0	-0.7364	3
12	4	10	19	0	0.4268	1
12	4	10	19	180	-0.7029	2
12	4	10	19	0	-0.7364	3
13	7	8	15	0	0.5941	1
13	7	8	15	180	-2.8995	2
13	7	8	15	0	0.6569	3
13	7	8	16	0	0.5941	1
13	7	8	16	180	-2.8995	2
13	7	8	16	0	0.6569	3
13	7	9	17	0	0.5941	1
13	7	9	17	180	-2.8995	2
13	7	9	17	0	0.6569	3
14	7	8	15	0	0.5941	1
14	7	8	15	180	-2.8995	2
14	7	8	15	0	0.6569	3
14	7	8	16	0	0.5941	1
14	7	8	16	180	-2.8995	2
14	7	8	16	0	0.6569	3
14	7	9	17	0	0.5941	1
14	7	9	17	180	-2.8995	2
14	7	9	17	0	0.6569	3
15	8	10	18	0	0.5941	1
15	8	10	18	180	-2.8995	2

15	8	10	18	0	0.6569	3
15	8	10	19	0	0.5941	1
15	8	10	19	180	-2.8995	2
15	8	10	19	0	0.6569	3
16	8	10	18	0	0.5941	1
16	8	10	18	180	-2.8995	2
16	8	10	18	0	0.6569	3
16	8	10	19	0	0.5941	1
16	8	10	19	180	-2.8995	2
16	8	10	19	0	0.6569	3
17	9	3	20	0	-0.318	1
17	9	3	20	180	-0.9205	2
17	9	3	20	0	0.7448	3
17	9	3	21	0	-0.318	1
17	9	3	21	180	-0.9205	2
17	9	3	21	0	0.7448	3

Improper

Atom Numbers				φ_0 / deg	k_ϕ / kJ mol^{-1} rad^{-2}
11	9	1	2	0	84.9101
9	7	11	3	0	0
9	3	11	17	0	0
7	8	9	13	0	0
7	13	9	14	0	0
8	10	7	16	0	0
16	7	15	0	0	2
10	4	8	18	0	0
10	4	8	19	0	0
12	5	4	6	0	34.3255
3	20	9	21	0	0
5	23	12	24	0	-4.2175
6	25	12	26	0	-4.2175



[Ga]

label	q	σ_{ii} / Å	ε_{ii} / kJ mol^{-1}	#
O3	-0.680071	3.15378	0.636386	1
O4	-0.666295	3.15378	0.636386	2
O5	-0.560035	3.02905	0.502080	3
O6	-0.573648	3.02905	0.502080	4
N5	-1.084913	3.29632	0.836800	5
C7	-0.477404	3.87541	0.230120	6
C8	0.519231	3.87541	0.230120	7

C9	-0.018317	3.87541	0.230120	8
C10	0.673511	3.56359	0.460240	9
C11	0.748918	3.56359	0.460240	10
H15	0.144424	2.35197	0.092048	11
H16	0.130487	2.35197	0.092048	12
H17	0.022099	2.35197	0.092048	13
H18	0.035553	2.35197	0.092048	14
H19	0.078646	2.35197	0.092048	15
H20	0.394158	0.40001	0.192464	16
H21	0.400242	0.40001	0.192464	17
H22	0.465901	0.40001	0.192464	18
H23	0.447513	0.40001	0.192464	19

Bonds

Atom Numbers		**r_{eq} /Å**	**k_r/ kJ mol^{-1} Å^{-2}**	
1	9	1.3550	1746.7195	-
1	18	0.9810	2229.0930	
2	10	1.3550	1746.7195	
2	19	0.9810	2229.0930	
3	9	1.2220	3899.3330	
4	10	1.2220	3899.3330	
5	7	1.4510	1530.8250	
5	16	1.0190	1954.1830	
5	17	1.0190	1954.1830	
6	7	1.5080	1282.1115	
6	8	1.5080	1282.1115	
6	12	1.0930	1435.0745	
6	11	1.0930	1435.0745	
7	9	1.4920	1261.6390	
7	13	1.0930	1435.0745	
8	10	1.4920	1261.6390	
8	15	1.0930	1435.0745	
8	14	1.0930	1435.0745	

Angles

Atom Numbers			**θ_{eq} / deg**	**k_θ / kJ mol^{-1} rad^{-2}**
9	1	18	111.948	351.09
10	2	19	111.948	351.09
7	5	16	109.062	459.49
7	5	17	109.062	459.49
16	5	17	105.998	358.32
7	6	8	109.608	512.48
7	6	11	110.549	383.00
7	6	12	110.549	383.00
8	6	11	110.549	383.00
8	6	12	110.549	383.00
11	6	12	108.836	310.74
5	7	6	108.29	467.91
5	7	9	105.837	720.84
5	7	13	110.297	393.25
6	7	9	107.517	467.91
6	7	13	110.549	383.00
9	7	13	108.385	391.44
6	8	10	107.517	467.91
6	8	14	110.549	383.00

6	8	15	110.549	383.00
10	8	14	108.385	391.44
10	8	15	108.385	391.44
14	8	15	108.836	310.74
1	9	3	124.425	695.55
1	9	7	109.716	628.10
3	9	7	124.41	564.87
2	10	4	124.425	695.55
2	10	8	109.716	628.10
4	10	8	124.41	564.87

Dihedrals

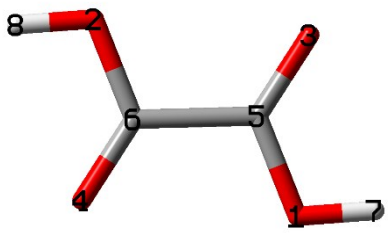
Atom Numbers				**δ / deg**	**k_ϕ / kJ mol^{-1}**	**m**
1	9	7	5	180	0.8368	2
1	9	7	5	0	0.6276	3
1	9	7	6	0	-0.2469	1
1	9	7	6	180	-0.6987	2
1	9	7	6	0	0.4226	3
1	9	7	13	180	-1.3054	2
1	9	7	13	0	0.6904	3
2	10	8	6	0	-0.2469	1
2	10	8	6	180	-0.6987	2
2	10	8	6	0	0.4226	3
2	10	8	14	180	-1.3054	2
2	10	8	14	0	0.6904	3
2	10	8	15	180	-1.3054	2
2	10	8	15	0	0.6904	3
3	9	1	18	0	3.4769	1
3	9	1	18	180	12.87	2
3	9	1	18	0	-0.1213	3
3	9	7	5	180	0.8368	2
3	9	7	5	0	0.8368	3
3	9	7	6	0	1.7238	1
3	9	7	6	180	0.2929	2
3	9	7	6	0	0.682	3
3	9	7	13	0	1.3807	1
3	9	7	13	180	-2.9455	2
3	9	7	13	0	0.6443	3
4	10	2	19	0	3.4769	1
4	10	2	19	180	12.87	2
4	10	2	19	0	-0.1213	3
4	10	8	6	0	1.7238	1
4	10	8	6	180	0.2929	2
4	10	8	6	0	0.682	3
4	10	8	14	0	1.3807	1
4	10	8	14	180	-2.9455	2
4	10	8	14	0	0.6443	3
4	10	8	15	0	1.3807	1
4	10	8	15	180	-2.9455	2
4	10	8	15	0	0.6443	3
5	7	6	8	0	-2.9706	1
5	7	6	8	180	-0.1925	2
5	7	6	8	0	2.3012	3
5	7	6	11	0	-1.5564	1
5	7	6	11	180	-2.5815	2

5	7	6	11	0	0.7071	3
5	7	6	12	0	-1.5564	1
5	7	6	12	180	-2.5815	2
5	7	6	12	0	0.7071	3
6	7	5	16	0	-0.8954	1
6	7	5	16	180	0.6778	2
6	7	5	16	0	0.5858	3
6	7	5	17	0	-0.8954	1
6	7	5	17	180	0.6778	2
6	7	5	17	0	0.5858	3
7	6	8	10	0	0.1381	1
7	6	8	10	180	-0.3264	2
7	6	8	10	0	0.2971	3
7	6	8	14	0	1.3389	1
7	6	8	14	180	-1.318	2
7	6	8	14	0	0.5523	3
7	6	8	15	0	1.3389	1
7	6	8	15	180	-1.318	2
7	6	8	15	0	0.5523	3
7	9	1	18	0	-2.4393	1
7	9	1	18	180	10.6232	2
7	9	1	18	0	-1.1422	3
8	6	7	9	0	0.1381	1
8	6	7	9	180	-0.3264	2
8	6	7	9	0	0.2971	3
8	6	7	13	0	1.3389	1
8	6	7	13	180	-1.318	2
8	6	7	13	0	0.5523	3
8	10	2	19	0	-2.4393	1
8	10	2	19	180	10.6232	2
8	10	2	19	0	-1.1422	3
9	7	5	16	180	-0.6276	2
9	7	5	16	0	1.046	3
9	7	5	17	180	-0.6276	2
9	7	5	17	0	1.046	3
9	7	6	11	0	-0.5356	1
9	7	6	11	180	0.1213	2
9	7	6	12	0	-0.5356	1
9	7	6	12	180	0.1213	2
10	8	6	11	0	-0.5356	1
10	8	6	11	180	0.1213	2
10	8	6	12	0	-0.5356	1
10	8	6	12	180	0.1213	2
11	6	7	13	0	0.5941	1
11	6	7	13	180	-2.8995	2
11	6	7	13	0	0.6569	3
11	6	8	14	0	0.5941	1
11	6	8	14	180	-2.8995	2
11	6	8	14	0	0.6569	3
11	6	8	15	0	0.5941	1
11	6	8	15	180	-2.8995	2
11	6	8	15	0	0.6569	3
12	6	7	13	0	0.5941	1
12	6	7	13	180	-2.8995	2
12	6	7	13	0	0.6569	3

12	6	8	14	0	0.5941	1
12	6	8	14	180	-2.8995	2
12	6	8	14	0	0.6569	3
12	6	8	15	0	0.5941	1
12	6	8	15	180	-2.8995	2
12	6	8	15	0	0.6569	3
13	7	5	16	0	-0.318	1
13	7	5	16	180	-0.9205	2
13	7	5	16	0	0.7448	3
13	7	5	17	0	-0.318	1
13	7	5	17	180	-0.9205	2
13	7	5	17	0	0.7448	3

Improper

	Atom Numbers			**φ_0 / deg**	**k_ϕ / kJ mol^{-1} rad^{-2}**
9	7	1	3	0	84.9101
7	6	9	5	0	0
7	5	9	13	0	0
6	8	7	12	0	0
6	8	7	11	0	0
8	10	6	15	0	0
8	10	6	14	0	0
10	2	8	4	0	84.9101
5	16	7	17	0	0



[Oa]

label	***q***	**σ_{ii} / Å**	**ε_{ii} / kJ mol^{-1}**	**#**
O3	-0.595908	3.15378	0.636386	1
O4	-0.594436	3.15378	0.636386	2
O5	-0.497392	3.02905	0.50208	3
O6	-0.495872	3.02905	0.50208	4
C7	0.643061	3.56359	0.46024	5
C8	0.638434	3.56359	0.46024	6
H15	0.451126	0.40001	0.192464	7
H16	0.450987	0.40001	0.192464	8

Bonds

Atom Numbers		r_{eq} /Å	k_r/ kJ mol^{-1} Å^{-2}
1	5	1.3550	1746.7195
1	7	0.9810	2229.0930
2	6	1.3550	1746.7195
2	8	0.9810	2229.0930
3	5	1.2220	3899.3330
4	6	1.2220	3899.3330
5	6	1.4890	1330.2900

Angles

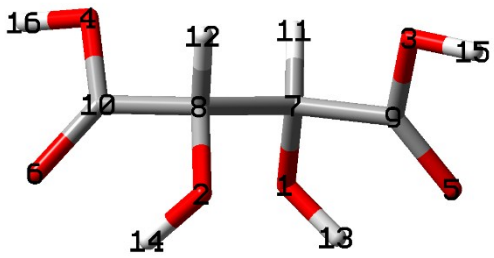
Atom Numbers			θ_{eq} / deg	k_θ / kJ mol^{-1} rad^{-2}
5	1	7	111.948	351.09
6	2	8	111.948	351.09
1	5	3	124.425	695.55
1	5	6	103.03	563.07
3	5	6	117.024	553.43
2	6	4	124.425	695.55
2	6	5	103.03	563.07
4	6	5	117.024	553.43

Dihedrals

Atom Numbers				δ / deg	k_ϕ / kJ mol^{-1}	m
1	5	6	2	0	0.5648	1
1	5	6	2	180	0.9121	2
1	5	6	4	0	-1.0334	1
1	5	6	4	180	1.661	2
1	5	6	4	0	-0.6653	3
2	6	5	3	0	-1.0334	1
2	6	5	3	180	1.661	2
2	6	5	3	0	-0.6653	3
3	5	1	7	0	3.4769	1
3	5	1	7	180	12.87	2
3	5	1	7	0	-0.1213	3
3	5	6	4	0	-0.5439	1
3	5	6	4	180	2.2677	2
3	5	6	4	0	0.4058	3
4	6	2	8	0	3.4769	1
4	6	2	8	180	12.87	2
4	6	2	8	0	-0.1213	3
5	6	2	8	0	3.4811	1
5	6	2	8	180	8.5228	2
5	6	2	8	0	0.1966	3
6	5	1	7	0	3.4811	1
6	5	1	7	180	8.5228	2
6	5	1	7	0	0.1966	3

Improper

Atom Numbers				φ_0 / deg	k_ϕ / kJ mol^{-1} rad^{-2}
5	6	1	3	0	76.4835
6	2	5	4	0	76.4835



[Ta]

label	*q*	σ_{ii} / Å	ε_{ii} / kJ mol^{-1}	#
O3	-0.629533	3.15378	0.636386	1
O4	-0.629180	3.15378	0.636386	2
O5	-0.627797	3.15378	0.636386	3
O6	-0.628310	3.15378	0.636386	4
O7	-0.524763	3.02905	0.502080	5
O8	-0.523755	3.02905	0.502080	6
C7	0.224155	3.87541	0.230120	7
C8	0.233523	3.87541	0.230120	8
C9	0.624321	3.56359	0.460240	9
C10	0.621721	3.56359	0.460240	10
H15	0.060469	2.35197	0.092048	11
H16	0.057581	2.35197	0.092048	12
H17	0.402418	0.40001	0.192464	13
H18	0.400789	0.40001	0.192464	14
H19	0.468969	0.40001	0.192464	15
H20	0.469390	0.40001	0.192464	16

Bonds

Atom Numbers		r_{eq} /Å	k_r/ kJ mol^{-1} Å^{-2}	
1	7	1.4180	1519.6875	-
1	13	0.9720	2346.8265	-
2	8	1.4180	1519.6875	-
2	14	0.9720	2346.8265	-
3	9	1.3550	1746.7195	-
3	15	0.9810	2229.0930	-
4	10	1.3550	1746.7195	-
4	16	0.9810	2229.0930	-
5	9	1.2220	3899.3330	-
6	10	1.2220	3899.3330	-
7	8	1.5080	1282.1115	-
7	9	1.4920	1261.6390	-
7	11	1.0930	1435.0745	-
8	10	1.4920	1261.6390	-
8	12	1.0930	1435.0745	-

Angles

Atom Numbers			θ_{eq} / deg	k_θ / kJ mol^{-1} rad^{-2}
7	1	13	106.503	477.55
8	2	14	106.503	477.55
9	3	15	111.948	351.09
10	4	16	111.948	351.09
1	7	8	108.133	597.39

1	7	9	104.112	317.97
1	7	11	108.577	470.32
8	7	9	107.517	467.91
8	7	11	110.549	383.00
9	7	11	108.385	391.44
2	8	7	108.133	597.39
2	8	10	104.112	317.97
2	8	12	108.577	470.32
7	8	10	107.517	467.91
7	8	12	110.549	383.00
10	8	12	108.385	391.44
3	9	5	124.425	695.55
3	9	7	109.716	628.10
5	9	7	124.41	564.87
4	10	6	124.425	695.55
4	10	8	109.716	628.10
6	10	8	124.41	564.87

Dihedrals

Atom Numbers				**δ / deg**	**k_ϕ / kJ mol^{-1}**	**m**
1	7	8	2	0	0.8535	1
1	7	8	2	180	2.9246	2
1	7	8	2	0	2.0083	3
1	7	8	10	0	-1.4226	1
1	7	8	10	180	-0.0628	2
1	7	8	12	0	-1.3682	1
1	7	8	12	180	2.2426	2
1	7	8	12	0	0.5858	3
1	7	9	3	0	0.9372	1
1	7	9	3	180	1.364	2
1	7	9	3	0	0.6653	3
1	7	9	5	0	-0.8284	1
1	7	9	5	180	1.5272	2
1	7	9	5	0	-0.2929	3
2	8	7	9	0	-1.4226	1
2	8	7	9	180	-0.0628	2
2	8	7	11	0	-1.3682	1
2	8	7	11	180	2.2426	2
2	8	7	11	0	0.5858	3
2	8	10	4	0	0.9372	1
2	8	10	4	180	1.364	2
2	8	10	4	0	0.6653	3
2	8	10	6	0	-0.8284	1
2	8	10	6	180	1.5272	2
2	8	10	6	0	-0.2929	3
3	9	7	8	0	-0.2469	1
3	9	7	8	180	-0.6987	2
3	9	7	8	0	0.4226	3
3	9	7	11	180	-1.3054	2
3	9	7	11	0	0.6904	3
4	10	8	7	0	-0.2469	1
4	10	8	7	180	-0.6987	2
4	10	8	7	0	0.4226	3
4	10	8	12	180	-1.3054	2
4	10	8	12	0	0.6904	3

5	9	3	15	0	3.4769	1
5	9	3	15	180	12.87	2
5	9	3	15	0	-0.1213	3
5	9	7	8	0	1.7238	1
5	9	7	8	180	0.2929	2
5	9	7	8	0	0.682	3
5	9	7	11	0	1.3807	1
5	9	7	11	180	-2.9455	2
5	9	7	11	0	0.6443	3
6	10	4	16	0	3.4769	1
6	10	4	16	180	12.87	2
6	10	4	16	0	-0.1213	3
6	10	8	7	0	1.7238	1
6	10	8	7	180	0.2929	2
6	10	8	7	0	0.682	3
6	10	8	12	0	1.3807	1
6	10	8	12	180	-2.9455	2
6	10	8	12	0	0.6443	3
7	8	2	14	180	0.5648	2
7	8	2	14	0	0.4937	3
7	9	3	15	0	-2.4393	1
7	9	3	15	180	10.6232	2
7	9	3	15	0	-1.1422	3
8	7	1	13	180	0.5648	2
8	7	1	13	0	0.4937	3
8	10	4	16	0	-2.4393	1
8	10	4	16	180	10.6232	2
8	10	4	16	0	-1.1422	3
9	7	1	13	0	-3.456	1
9	7	1	13	180	-3.4727	2
9	7	1	13	0	0.5899	3
9	7	8	10	0	0.9288	1
9	7	8	10	0	-2.3849	3
9	7	8	12	0	-0.5356	1
9	7	8	12	180	0.1213	2
10	8	2	14	0	-3.456	1
10	8	2	14	180	-3.4727	2
10	8	2	14	0	0.5899	3
10	8	7	11	0	-0.5356	1
10	8	7	11	180	0.1213	2
11	7	1	13	0	1.2468	1
11	7	1	13	180	-0.5774	2
11	7	1	13	0	0.7238	3
11	7	8	12	0	0.5941	1
11	7	8	12	180	-2.8995	2
11	7	8	12	0	0.6569	3
12	8	2	14	0	1.2468	1
12	8	2	14	180	-0.5774	2
12	8	2	14	0	0.7238	3

Improper

Atom Numbers				φ_0 / deg	k_ϕ / kJ mol^{-1} rad^{-2}
7	8	1	9	0	0
7	8	1	11	0	0
8	10	7	2	0	0
2	7	12	0	0	0
3	7	5	0	0	84.9101
10	4	8	6	0	84.9101

Table S2. Systems used for MD simulations of Ld + DES (Ar:Ga,Oa,Ta). x_{Ld} stands for Ld mole fraction, N_i for the number of *i-molecules*

x_{Ld}	N_{Ar}	$N_{Ga\,/\,Oa\,/\,Ta}$	N_{Ld}	T / K	P / bar
0	500	500	0	298	1
0.1	500	500	56	298	1
0.2	500	500	125	298	1
0.3	500	500	214	298	1
0.4	500	500	333	298	1
0.5	500	500	500	298	1

Table S3. Studied DES geometry optimization positions and their final SCF energy values.

DES	Position	ORCA Total SCF Energy (eH)
ArGa	p01	-1157.93235780
	p02	-1157.93265269
	p03	-1157.92290555
	p04	-1157.92336690
ArOa	p01	-984.68993790
	p02	-984.68143699
	p03	-984.68144344
ArTa	p01	-1213.72440486
	p02	-1213.71573448
	p04	-1213.71136459
	p05	-1213.70392747

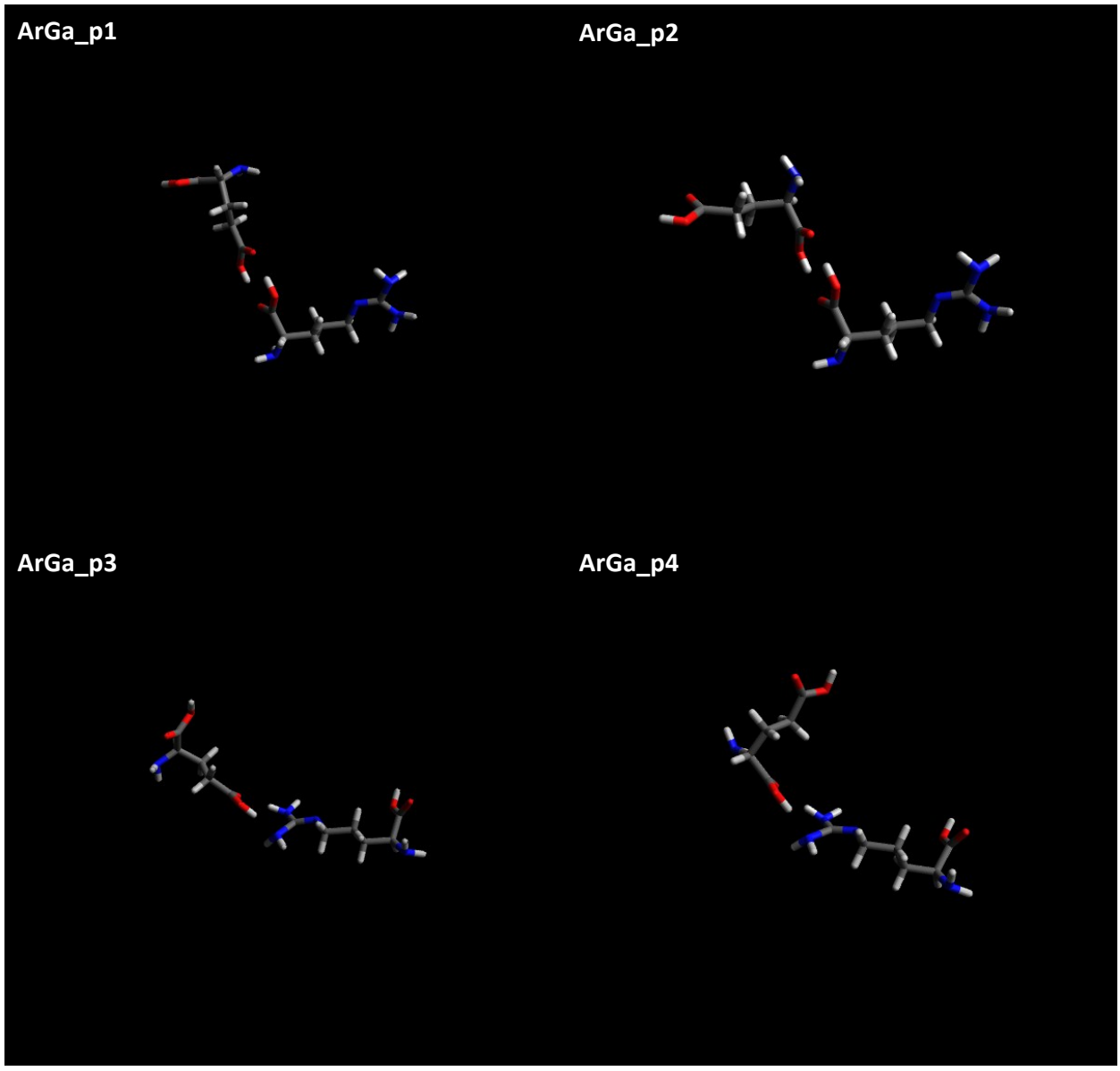


Fig. S1 DFT geometry optimization simulation results for all studied ArGa DES structures.

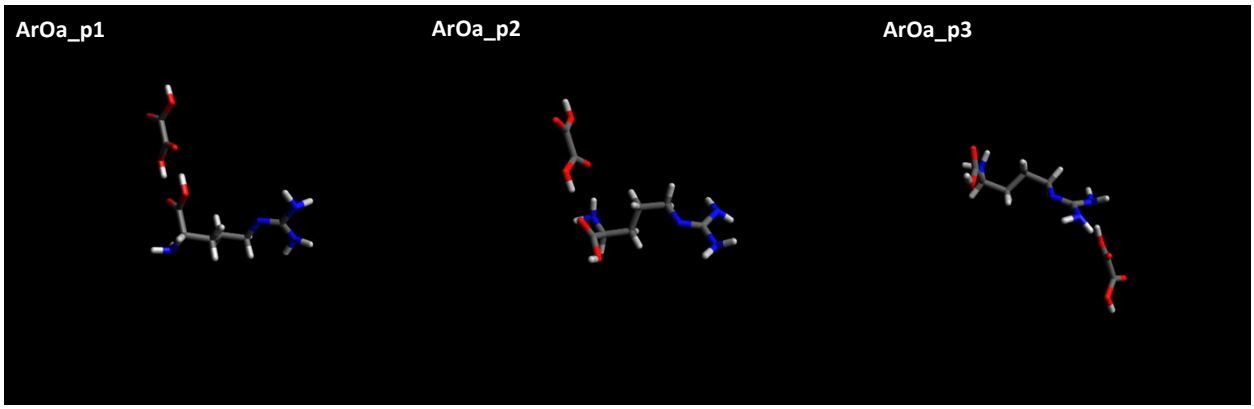


Fig. S2 DFT geometry optimization simulation results for all studied ArOa DES structures.

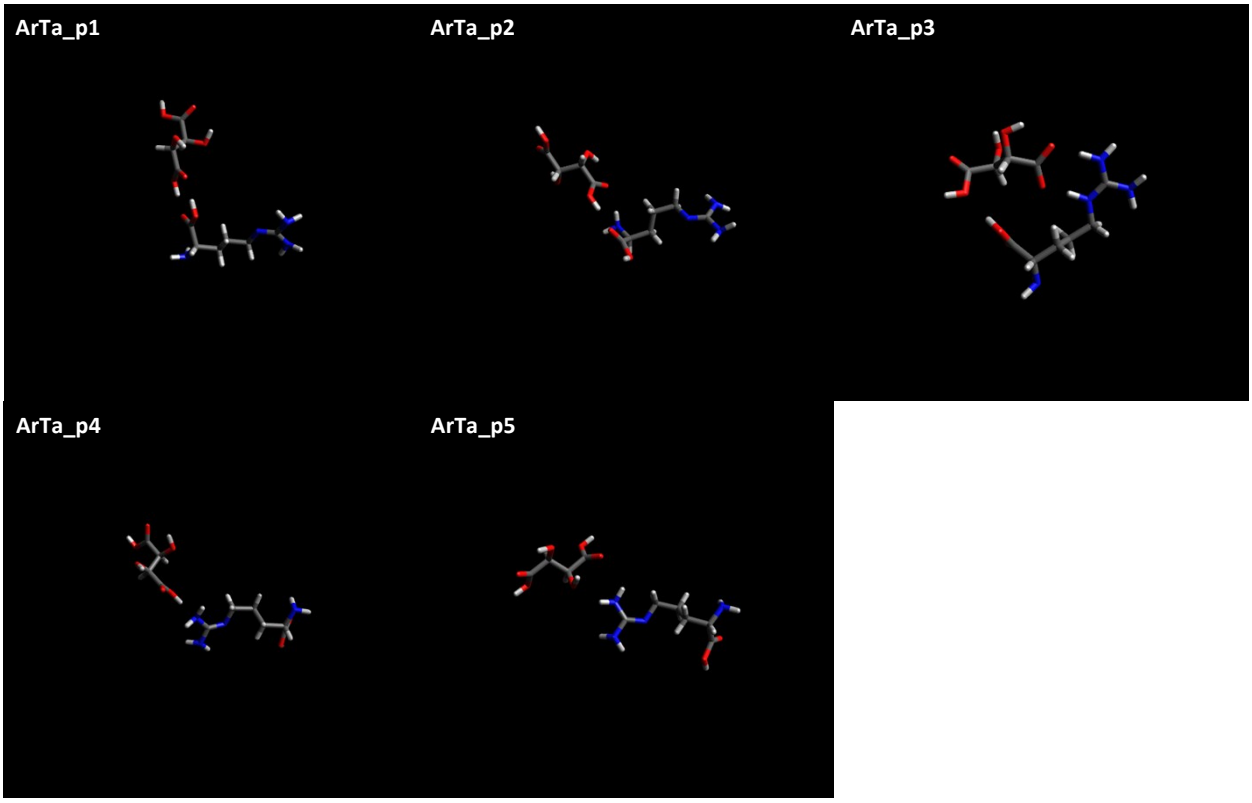


Fig. S3 DFT geometry optimization simulation results for all studied ArTa DES structures.

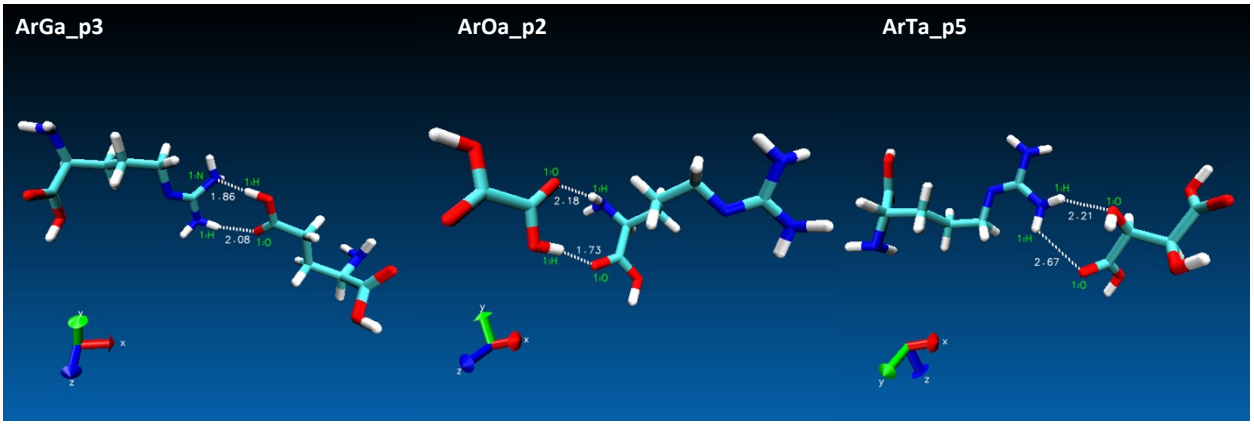


Fig. S4 Lowest energy ArGa, ArOa and ArTa structures

References

1 A. Gutiérrez, M. Atilhan, S. Aparicio, A theoretical study on lidocaine solubility in deep eutectic solvents, *Phys. Chem. Chem. Phys.* 2018, **20**, 27464-27473.