Supporting Information

A Theoretical Study on Deep Eutectic Solvents as Vehicles for Anesthetics Delivery

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Table S1. Forcefield parameterizations for compounds 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:

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

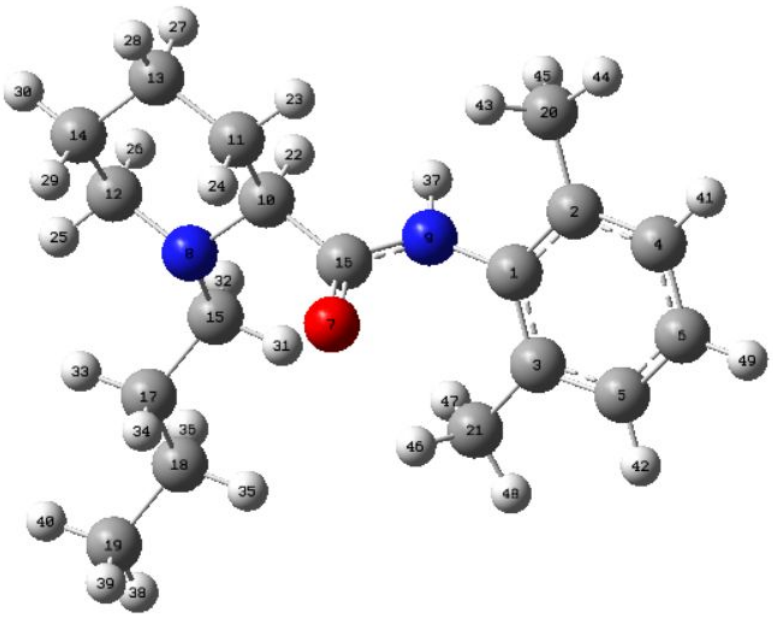
Improper dihedrals were described according to:

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

DESs

These compounds were described according to the forcefield reported in a previous work (Ref. 1)

ANESTHETICS



Bp

Atoms

q	σ_{ii} / Å	ε_{ii}/ kJ mol^{-1}	#
0.029676	3.55005	0.29288	1
0.380610	3.55005	0.29288	2
0.228535	3.55005	0.29288	3
-0.410375	3.55005	0.29288	4
-0.338863	3.55005	0.29288	5
-0.079130	3.55005	0.29288	6
-0.564711	3.02905	0.50208	7

-0.428226	3.29632	0.83680	8
-0.582105	3.29632	0.83680	9
-0.001778	3.87541	0.23012	10
-0.161322	3.87541	0.23012	11
0.130742	3.87541	0.23012	12
0.102613	3.87541	0.23012	13
-0.153139	3.87541	0.23012	14
-0.106159	3.87541	0.23012	15
0.731832	3.56359	0.46024	16
0.048986	3.87541	0.23012	17
0.177405	3.87541	0.23012	18
-0.372338	3.87541	0.23012	19
-0.590133	3.87541	0.23012	20
-0.389028	3.87541	0.23012	21
0.051488	2.35197	0.09205	22
0.028385	2.35197	0.09205	23
0.091594	2.35197	0.09205	24
0.044366	2.35197	0.09205	25
0.020720	2.35197	0.09205	26
-0.007030	2.35197	0.09205	27
0.002329	2.35197	0.09205	28
0.068741	2.35197	0.09205	29
0.029035	2.35197	0.09205	30
0.081102	2.35197	0.09205	31
0.028070	2.35197	0.09205	32
0.025267	2.35197	0.09205	33
0.026295	2.35197	0.09205	34
-0.019121	2.35197	0.09205	35
-0.029243	2.35197	0.09205	36
0.294795	0.40001	0.19246	37
0.092517	2.35197	0.09205	38
0.080915	2.35197	0.09205	39
0.076818	2.35197	0.09205	40
0.190509	2.35197	0.09205	41
0.178817	2.35197	0.09205	42
0.174194	2.35197	0.09205	43
0.155487	2.35197	0.09205	44
0.145924	2.35197	0.09205	45
0.176026	2.35197	0.09205	46
0.097501	2.35197	0.09205	47
0.099187	2.35197	0.09205	48
0.142221	2.35197	0.09205	49

Bonds

Atom Numbers		**r_{eq} /Å**	**k_r/ kJ mol^{-1} Å^{-2}**
7	16	1.222	3899.3330
8	10	1.451	1530.8250
8	12	1.451	1530.8250
8	15	1.451	1530.8250
9	16	1.369	1755.1505
9	1	1.395	1650.6675
9	37	1.015	2006.2740
10	11	1.508	1282.1115
10	16	1.492	1261.6390
10	22	1.093	1435.0745
11	13	1.508	1282.1115
11	23	1.093	1435.0745

11	24	1.093	1435.0745
12	14	1.508	1282.1115
12	25	1.093	1435.0745
12	26	1.093	1435.0745
13	14	1.508	1282.1115
13	27	1.093	1435.0745
13	28	1.093	1435.0745
14	29	1.093	1435.0745
14	30	1.093	1435.0745
15	17	1.508	1282.1115
15	31	1.093	1435.0745
15	32	1.093	1435.0745
17	18	1.508	1282.1115
17	33	1.093	1435.0745
17	34	1.093	1435.0745
18	19	1.508	1282.1115
18	35	1.093	1435.0745
18	36	1.093	1435.0745
1	2	1.374	1678.0685
1	3	1.374	1678.0685
19	38	1.093	1435.0745
19	39	1.093	1435.0745
19	40	1.093	1435.0745
2	4	1.374	1678.0685
2	20	1.486	1492.5875
3	5	1.374	1678.0685
3	21	1.486	1492.5875
4	6	1.374	1678.0685
4	41	1.084	1597.6730
5	6	1.374	1678.0685
5	42	1.084	1597.6730
20	43	1.093	1435.0745
20	44	1.093	1435.0745
20	45	1.093	1435.0745
21	46	1.093	1435.0745
21	47	1.093	1435.0745
21	48	1.093	1435.0745
6	49	1.084	1597.6730

Angles

Atom Numbers			**θ_{eq} / deg**	**k_θ / kJ mol^{-1} rad^{-2}**
2	1	3	119.977	402.88
2	1	9	117.918	617.27
3	1	9	117.918	617.27
1	2	4	119.977	402.88
1	2	20	120.419	483.57
4	2	20	120.419	483.57
1	3	5	119.977	402.88
1	3	21	120.419	483.57
5	3	21	120.419	483.57
2	4	6	119.977	402.88
2	4	41	120.571	339.05
6	4	41	120.571	339.05
3	5	6	119.977	402.88
3	5	42	120.571	339.05
6	5	42	120.571	339.05
4	6	5	119.977	402.88

4	6	49	120.571	339.05
5	6	49	120.571	339.05
10	8	12	107.018	656.41
10	8	15	107.018	656.41
12	8	15	107.018	656.41
1	9	16	118.596	616.06
1	9	37	118.227	378.18
16	9	37	120.277	346.27
8	10	11	108.290	467.91
8	10	16	105.837	720.84
8	10	22	110.297	393.25
11	10	16	107.517	467.91
11	10	22	110.549	383.00
16	10	22	108.385	391.44
10	11	13	109.608	512.48
10	11	23	110.549	383.00
10	11	24	110.549	383.00
13	11	23	110.549	383.00
13	11	24	110.549	383.00
23	11	24	108.836	310.74
8	12	14	108.290	467.91
8	12	25	110.297	393.25
8	12	26	110.297	393.25
14	12	25	110.549	383.00
14	12	26	110.549	383.00
25	12	26	108.836	310.74
11	13	14	109.608	512.48
11	13	27	110.549	383.00
11	13	28	110.549	383.00
14	13	27	110.549	383.00
14	13	28	110.549	383.00
27	13	28	108.836	310.74
12	14	13	109.608	512.48
12	14	29	110.549	383.00
12	14	30	110.549	383.00
13	14	29	110.549	383.00
13	14	30	110.549	383.00
29	14	30	108.836	310.74
8	15	17	108.290	467.91
8	15	31	110.297	393.25
8	15	32	110.297	393.25
17	15	31	110.549	383.00
17	15	32	110.549	383.00
31	15	32	108.836	310.74
7	16	9	127.152	546.20
7	16	10	124.410	564.87
9	16	10	112.735	592.57
15	17	18	109.608	512.48
15	17	33	110.549	383.00
15	17	34	110.549	383.00
18	17	33	110.549	383.00
18	17	34	110.549	383.00
33	17	34	108.836	310.74
17	18	19	109.608	512.48
17	18	35	110.549	383.00
17	18	36	110.549	383.00
19	18	35	110.549	383.00

19	18	36	110.549	383.00
35	18	36	108.836	310.74
18	19	38	110.549	383.00
18	19	39	110.549	383.00
18	19	40	110.549	383.00
38	19	39	108.836	310.74
38	19	40	108.836	310.74
39	19	40	108.836	310.74
2	20	43	109.491	377.58
2	20	44	109.491	377.58
2	20	45	109.491	377.58
43	20	44	108.836	310.74
43	20	45	108.836	310.74
44	20	45	108.836	310.74
3	21	46	109.491	377.58
3	21	47	109.491	377.58
3	21	48	109.491	377.58
46	21	47	108.836	310.74
46	21	48	108.836	310.74
47	21	48	108.836	310.74

Dihedrals

Atom Numbers				**δ / deg**	**k_ϕ / kJ mol^{-1}**	**m**
1	2	4	6	180	14.644	2
1	2	4	41	180	14.644	2
1	2	20	43	180	-0.8786	2
1	2	20	43	0	0.8201	3
1	2	20	44	180	-0.8786	2
1	2	20	44	0	0.8201	3
1	2	20	45	180	-0.8786	2
1	2	20	45	0	0.8201	3
1	3	5	6	180	14.644	2
1	3	5	42	180	14.644	2
1	3	21	46	180	-0.8786	2
1	3	21	46	0	0.8201	3
1	3	21	47	180	-0.8786	2
1	3	21	47	0	0.8201	3
1	3	21	48	180	-0.8786	2
1	3	21	48	0	0.8201	3
1	9	16	7	180	12.552	2
1	9	16	10	180	12.552	2
2	1	3	5	180	14.644	2
2	1	3	21	180	14.644	2
2	1	9	16	180	12.552	2
2	1	9	37	180	12.552	2
2	4	6	5	180	14.644	2
2	4	6	49	180	14.644	2
3	1	2	4	180	14.644	2
3	1	2	20	180	14.644	2
3	1	9	16	180	12.552	2
3	1	9	37	180	12.552	2
3	5	6	4	180	14.644	2
3	5	6	49	180	14.644	2
4	2	1	9	180	14.644	2
4	2	20	43	180	-0.8786	2
4	2	20	43	0	0.8201	3
4	2	20	44	180	-0.8786	2

4	2	20	44	0	0.8201	3
4	2	20	45	180	-0.8786	2
4	2	20	45	0	0.8201	3
4	6	5	42	180	14.644	2
5	3	1	9	180	14.644	2
5	3	21	46	180	-0.8786	2
5	3	21	46	0	0.8201	3
5	3	21	47	180	-0.8786	2
5	3	21	47	0	0.8201	3
5	3	21	48	180	-0.8786	2
5	3	21	48	0	0.8201	3
5	6	4	41	180	14.644	2
6	4	2	20	180	14.644	2
6	5	3	21	180	14.644	2
7	16	9	37	0	3.0041	1
7	16	9	37	180	10.4056	2
7	16	9	37	0	-0.9498	3
7	16	10	8	180	0.8368	2
7	16	10	8	0	0.8368	3
7	16	10	11	0	1.7238	1
7	16	10	11	180	0.2929	2
7	16	10	11	0	0.682	3
7	16	10	22	0	1.3807	1
7	16	10	22	180	-2.9455	2
7	16	10	22	0	0.6443	3
8	10	11	13	0	-2.9706	1
8	10	11	13	180	-0.1925	2
8	10	11	13	0	2.3012	3
8	10	11	23	0	-1.5564	1
8	10	11	23	180	-2.5815	2
8	10	11	23	0	0.7071	3
8	10	11	24	0	-1.5564	1
8	10	11	24	180	-2.5815	2
8	10	11	24	0	0.7071	3
8	10	16	9	180	0.8368	2
8	10	16	9	0	0.6276	3
8	12	14	13	0	-2.9706	1
8	12	14	13	180	-0.1925	2
8	12	14	13	0	2.3012	3
8	12	14	29	0	-1.5564	1
8	12	14	29	180	-2.5815	2
8	12	14	29	0	0.7071	3
8	12	14	30	0	-1.5564	1
8	12	14	30	180	-2.5815	2
8	12	14	30	0	0.7071	3
8	15	17	18	0	-2.9706	1
8	15	17	18	180	-0.1925	2
8	15	17	18	0	2.3012	3
8	15	17	33	0	-1.5564	1
8	15	17	33	180	-2.5815	2
8	15	17	33	0	0.7071	3
8	15	17	34	0	-1.5564	1
8	15	17	34	180	-2.5815	2
8	15	17	34	0	0.7071	3
9	1	2	20	180	14.644	2
9	1	3	21	180	14.644	2
9	16	10	11	0	-1.9414	1

9	16	10	11	180	2.3263	2
9	16	10	11	0	2.9037	3
9	16	10	22	0	-0.8619	1
9	16	10	22	180	1.4477	2
9	16	10	22	0	0.1799	3
10	8	12	14	0	-0.9205	1
10	8	12	14	180	1.6443	2
10	8	12	14	0	0.569	3
10	8	12	25	0	0.8242	1
10	8	12	25	180	-0.8075	2
10	8	12	25	0	1.1757	3
10	8	12	26	0	0.8242	1
10	8	12	26	180	-0.8075	2
10	8	12	26	0	1.1757	3
10	8	15	17	0	-0.9205	1
10	8	15	17	180	1.6443	2
10	8	15	17	0	0.569	3
10	8	15	31	0	0.8242	1
10	8	15	31	180	-0.8075	2
10	8	15	31	0	1.1757	3
10	8	15	32	0	0.8242	1
10	8	15	32	180	-0.8075	2
10	8	15	32	0	1.1757	3
10	11	13	14	0	0.2134	1
10	11	13	14	180	1.4267	2
10	11	13	14	0	0.6945	3
10	11	13	27	0	1.3389	1
10	11	13	27	180	-1.318	2
10	11	13	27	0	0.5523	3
10	11	13	28	0	1.3389	1
10	11	13	28	180	-1.318	2
10	11	13	28	0	0.5523	3
10	16	9	37	0	-0.615	1
10	16	9	37	180	12.142	2
10	16	9	37	0	2.8075	3
11	10	8	12	0	-0.9205	1
11	10	8	12	180	1.6443	2
11	10	8	12	0	0.569	3
11	10	8	15	0	-0.9205	1
11	10	8	15	180	1.6443	2
11	10	8	15	0	0.569	3
11	13	14	12	0	0.2134	1
11	13	14	12	180	1.4267	2
11	13	14	12	0	0.6945	3
11	13	14	29	0	1.3389	1
11	13	14	29	180	-1.318	2
11	13	14	29	0	0.5523	3
11	13	14	30	0	1.3389	1
11	13	14	30	180	-1.318	2
11	13	14	30	0	0.5523	3
12	8	10	16	180	-0.6276	2
12	8	10	16	0	1.046	3
12	8	10	22	0	0.8242	1
12	8	10	22	180	-0.8075	2
12	8	10	22	0	1.1757	3
12	8	15	17	0	-0.9205	1
12	8	15	17	180	1.6443	2

12	8	15	17	0	0.569	3
12	8	15	31	0	0.8242	1
12	8	15	31	180	-0.8075	2
12	8	15	31	0	1.1757	3
12	8	15	32	0	0.8242	1
12	8	15	32	180	-0.8075	2
12	8	15	32	0	1.1757	3
12	14	13	27	0	1.3389	1
12	14	13	27	180	-1.318	2
12	14	13	27	0	0.5523	3
12	14	13	28	0	1.3389	1
12	14	13	28	180	-1.318	2
12	14	13	28	0	0.5523	3
13	11	10	16	0	0.1381	1
13	11	10	16	180	-0.3264	2
13	11	10	16	0	0.2971	3
13	11	10	22	0	1.3389	1
13	11	10	22	180	-1.318	2
13	11	10	22	0	0.5523	3
13	14	12	25	0	1.3389	1
13	14	12	25	180	-1.318	2
13	14	12	25	0	0.5523	3
13	14	12	26	0	1.3389	1
13	14	12	26	180	-1.318	2
13	14	12	26	0	0.5523	3
14	12	8	15	0	-0.9205	1
14	12	8	15	180	1.6443	2
14	12	8	15	0	0.569	3
14	13	11	23	0	1.3389	1
14	13	11	23	180	-1.318	2
14	13	11	23	0	0.5523	3
14	13	11	24	0	1.3389	1
14	13	11	24	180	-1.318	2
14	13	11	24	0	0.5523	3
15	8	10	16	180	-0.6276	2
15	8	10	16	0	1.046	3
15	8	10	22	0	0.8242	1
15	8	10	22	180	-0.8075	2
15	8	10	22	0	1.1757	3
15	8	12	25	0	0.8242	1
15	8	12	25	180	-0.8075	2
15	8	12	25	0	1.1757	3
15	8	12	26	0	0.8242	1
15	8	12	26	180	-0.8075	2
15	8	12	26	0	1.1757	3
15	17	18	19	0	0.2134	1
15	17	18	19	180	1.4267	2
15	17	18	19	0	0.6945	3
15	17	18	35	0	1.3389	1
15	17	18	35	180	-1.318	2
15	17	18	35	0	0.5523	3
15	17	18	36	0	1.3389	1
15	17	18	36	180	-1.318	2
15	17	18	36	0	0.5523	3
16	10	11	23	0	-0.5356	1
16	10	11	23	180	0.1213	2
16	10	11	24	0	-0.5356	1

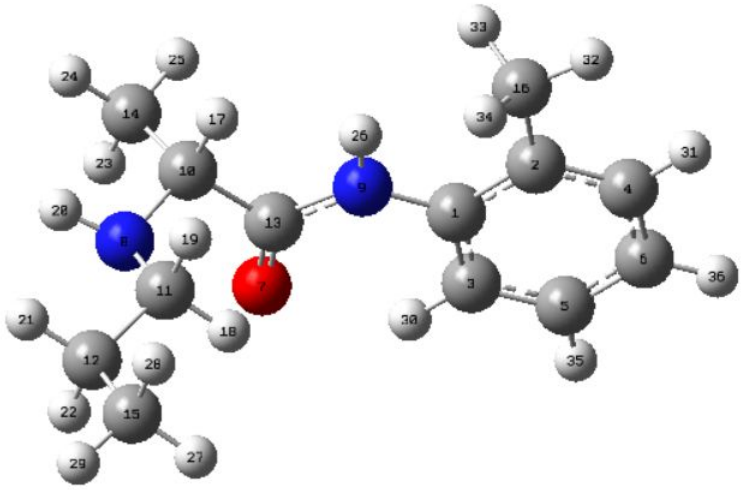
16	10	11	24	180	0.1213	2
17	18	19	38	0	1.3389	1
17	18	19	38	180	-1.318	2
17	18	19	38	0	0.5523	3
17	18	19	39	0	1.3389	1
17	18	19	39	180	-1.318	2
17	18	19	39	0	0.5523	3
17	18	19	40	0	1.3389	1
17	18	19	40	180	-1.318	2
17	18	19	40	0	0.5523	3
18	17	15	31	0	1.3389	1
18	17	15	31	180	-1.318	2
18	17	15	31	0	0.5523	3
18	17	15	32	0	1.3389	1
18	17	15	32	180	-1.318	2
18	17	15	32	0	0.5523	3
19	18	17	33	0	1.3389	1
19	18	17	33	180	-1.318	2
19	18	17	33	0	0.5523	3
19	18	17	34	0	1.3389	1
19	18	17	34	180	-1.318	2
19	18	17	34	0	0.5523	3
20	2	4	41	180	14.644	2
21	3	5	42	180	14.644	2
22	10	11	23	0	0.5941	1
22	10	11	23	180	-2.8995	2
22	10	11	23	0	0.6569	3
22	10	11	24	0	0.5941	1
22	10	11	24	180	-2.8995	2
22	10	11	24	0	0.6569	3
23	11	13	27	0	0.5941	1
23	11	13	27	180	-2.8995	2
23	11	13	27	0	0.6569	3
23	11	13	28	0	0.5941	1
23	11	13	28	180	-2.8995	2
23	11	13	28	0	0.6569	3
24	11	13	27	0	0.5941	1
24	11	13	27	180	-2.8995	2
24	11	13	27	0	0.6569	3
24	11	13	28	0	0.5941	1
24	11	13	28	180	-2.8995	2
24	11	13	28	0	0.6569	3
25	12	14	29	0	0.5941	1
25	12	14	29	180	-2.8995	2
25	12	14	29	0	0.6569	3
25	12	14	30	0	0.5941	1
25	12	14	30	180	-2.8995	2
25	12	14	30	0	0.6569	3
26	12	14	29	0	0.5941	1
26	12	14	29	180	-2.8995	2
26	12	14	29	0	0.6569	3
26	12	14	30	0	0.5941	1
26	12	14	30	180	-2.8995	2
26	12	14	30	0	0.6569	3
27	13	14	29	0	0.5941	1
27	13	14	29	180	-2.8995	2
27	13	14	29	0	0.6569	3

27	13	14	30	0	0.5941	1
27	13	14	30	180	-2.8995	2
27	13	14	30	0	0.6569	3
28	13	14	29	0	0.5941	1
28	13	14	29	180	-2.8995	2
28	13	14	29	0	0.6569	3
28	13	14	30	0	0.5941	1
28	13	14	30	180	-2.8995	2
28	13	14	30	0	0.6569	3
31	15	17	33	0	0.5941	1
31	15	17	33	180	-2.8995	2
31	15	17	33	0	0.6569	3
31	15	17	34	0	0.5941	1
31	15	17	34	180	-2.8995	2
31	15	17	34	0	0.6569	3
32	15	17	33	0	0.5941	1
32	15	17	33	180	-2.8995	2
32	15	17	33	0	0.6569	3
32	15	17	34	0	0.5941	1
32	15	17	34	180	-2.8995	2
32	15	17	34	0	0.6569	3
33	17	18	35	0	0.5941	1
33	17	18	35	180	-2.8995	2
33	17	18	35	0	0.6569	3
33	17	18	36	0	0.5941	1
33	17	18	36	180	-2.8995	2
33	17	18	36	0	0.6569	3
34	17	18	35	0	0.5941	1
34	17	18	35	180	-2.8995	2
34	17	18	35	0	0.6569	3
34	17	18	36	0	0.5941	1
34	17	18	36	180	-2.8995	2
34	17	18	36	0	0.6569	3
35	18	19	38	0	0.5941	1
35	18	19	38	180	-2.8995	2
35	18	19	38	0	0.6569	3
35	18	19	39	0	0.5941	1
35	18	19	39	180	-2.8995	2
35	18	19	39	0	0.6569	3
35	18	19	40	0	0.5941	1
35	18	19	40	180	-2.8995	2
35	18	19	40	0	0.6569	3
36	18	19	38	0	0.5941	1
36	18	19	38	180	-2.8995	2
36	18	19	38	0	0.6569	3
36	18	19	39	0	0.5941	1
36	18	19	39	180	-2.8995	2
36	18	19	39	0	0.6569	3
36	18	19	40	0	0.5941	1
36	18	19	40	180	-2.8995	2
36	18	19	40	0	0.6569	3
41	4	6	49	180	14.644	2
42	5	6	49	180	14.644	2

Improper

Atom Numbers				**φ_0 / deg**	**k_ϕ / kJ mol^{-1} rad^{-2}**
1	3	9	2	0	21.079

2	4	1	20	0	24.0915
3	5	1	21	0	24.0915
4	6	2	41	0	9.0291
9	16	1	37	0	-12.0416
16	10	9	7	0	77.6885
10	8	16	11	0	0
10	8	16	22	0	0
8	15	10	12	0	0
11	13	10	23	0	0
11	13	10	24	0	0
12	14	8	25	0	0
12	14	8	26	0	0
15	17	8	31	0	0
15	17	8	32	0	0
17	18	15	33	0	0
17	18	15	34	0	0
18	19	17	35	0	0
18	19	17	36	0	0
13	14	11	27	0	0
13	14	11	28	0	0
14	13	12	29	0	0
14	13	12	30	0	0
19	38	18	39	0	0
19	38	18	40	0	0
5	6	3	42	0	9.0291
20	43	2	44	0	0
20	43	2	45	0	0
21	46	3	47	0	0
21	46	3	48	0	0
6	5	4	49	0	9.0291



Pl

Atoms

q	σ_{ii} / Å	ε_{ii}/ kJ mol^{-1}	#
0.366916	3.55005	0.29288	1
0.195950	3.55005	0.29288	2
-0.291129	3.55005	0.29288	3
-0.311738	3.55005	0.29288	4
-0.164459	3.55005	0.29288	5

-0.146759	3.55005	0.29288	6
-0.589961	3.02905	0.50208	7
-0.898265	3.29632	0.83680	8
-0.775432	3.29632	0.83680	9
0.310545	3.87541	0.23012	10
0.250479	3.87541	0.23012	11
0.223115	3.87541	0.23012	12
0.861762	3.56359	0.46024	13
-0.576738	3.87541	0.23012	14
-0.423467	3.87541	0.23012	15
-0.461804	3.87541	0.23012	16
0.006642	2.35197	0.09205	17
0.025461	2.35197	0.09205	18
-0.049520	2.35197	0.09205	19
0.376739	0.40001	0.19246	20
-0.030015	2.35197	0.09205	21
-0.009993	2.35197	0.09205	22
0.172565	2.35197	0.09205	23
0.159877	2.35197	0.09205	24
0.125242	2.35197	0.09205	25
0.294607	0.40001	0.19246	26
0.092107	2.35197	0.09205	27
0.086908	2.35197	0.09205	28
0.106365	2.35197	0.09205	29
0.215234	2.35197	0.09205	30
0.174570	2.35197	0.09205	31
0.140682	2.35197	0.09205	32
0.128769	2.35197	0.09205	33
0.123001	2.35197	0.09205	34
0.148985	2.35197	0.09205	35
0.142758	2.35197	0.09205	36

Bonds

Atom Numbers		**r_{eq} /Å**	**k_r/ kJ mol^{-1} Å^{-2}**
7	13	1.222	3899.3330
8	10	1.451	1530.8250
8	11	1.451	1530.8250
8	20	1.019	1954.1830
9	13	1.369	1755.1505
9	1	1.395	1650.6675
9	26	1.015	2006.2740
10	13	1.492	1261.6390
10	14	1.508	1282.1115
10	17	1.093	1435.0745
11	12	1.508	1282.1115
11	18	1.093	1435.0745
11	19	1.093	1435.0745
12	15	1.508	1282.1115
12	21	1.093	1435.0745
12	22	1.093	1435.0745
14	23	1.093	1435.0745
14	24	1.093	1435.0745
14	25	1.093	1435.0745
1	2	1.374	1678.0685
1	3	1.374	1678.0685
2	4	1.374	1678.0685
2	16	1.486	1492.5875

15	27	1.093	1435.0745
15	28	1.093	1435.0745
15	29	1.093	1435.0745
3	5	1.374	1678.0685
3	30	1.084	1597.6730
4	6	1.374	1678.0685
4	31	1.084	1597.6730
16	32	1.093	1435.0745
16	33	1.093	1435.0745
16	34	1.093	1435.0745
5	6	1.374	1678.0685
5	35	1.084	1597.6730
6	36	1.084	1597.6730

Angles

Atom Numbers			**θ_{eq} / deg**	**k_θ / kJ mol^{-1} rad^{-2}**
2	1	3	119.977	402.88
2	1	9	117.918	617.27
3	1	9	117.918	617.27
1	2	4	119.977	402.88
1	2	16	120.419	483.57
4	2	16	120.419	483.57
1	3	5	119.977	402.88
1	3	30	120.571	339.05
5	3	30	120.571	339.05
2	4	6	119.977	402.88
2	4	31	120.571	339.05
6	4	31	120.571	339.05
3	5	6	119.977	402.88
3	5	35	120.571	339.05
6	5	35	120.571	339.05
4	6	5	119.977	402.88
4	6	36	120.571	339.05
5	6	36	120.571	339.05
10	8	11	107.018	656.41
10	8	20	109.062	459.49
11	8	20	109.062	459.49
1	9	13	118.596	616.06
1	9	26	118.227	378.18
13	9	26	120.277	346.27
8	10	13	105.837	720.84
8	10	14	108.290	467.91
8	10	17	110.297	393.25
13	10	14	107.517	467.91
13	10	17	108.385	391.44
14	10	17	110.549	383.00
8	11	12	108.290	467.91
8	11	18	110.297	393.25
8	11	19	110.297	393.25
12	11	18	110.549	383.00
12	11	19	110.549	383.00
18	11	19	108.836	310.74
11	12	15	109.608	512.48
11	12	21	110.549	383.00
11	12	22	110.549	383.00
15	12	21	110.549	383.00
15	12	22	110.549	383.00

21	12	22	108.836	310.74
7	13	9	127.152	546.20
7	13	10	124.410	564.87
9	13	10	112.735	592.57
10	14	23	110.549	383.00
10	14	24	110.549	383.00
10	14	25	110.549	383.00
23	14	24	108.836	310.74
23	14	25	108.836	310.74
24	14	25	108.836	310.74
12	15	27	110.549	383.00
12	15	28	110.549	383.00
12	15	29	110.549	383.00
27	15	28	108.836	310.74
27	15	29	108.836	310.74
28	15	29	108.836	310.74
2	16	32	109.491	377.58
2	16	33	109.491	377.58
2	16	34	109.491	377.58
32	16	33	108.836	310.74
32	16	34	108.836	310.74
33	16	34	108.836	310.74

Dihedrals

Atom Numbers				**δ / deg**	**k_ϕ / kJ mol^{-1}**	**m**
1	2	4	6	180	14.644	2
1	2	4	31	180	14.644	2
1	2	16	32	180	-0.8786	2
1	2	16	32	0	0.8201	3
1	2	16	33	180	-0.8786	2
1	2	16	33	0	0.8201	3
1	2	16	34	180	-0.8786	2
1	2	16	34	0	0.8201	3
1	3	5	6	180	14.644	2
1	3	5	35	180	14.644	2
1	9	13	7	180	12.552	2
1	9	13	10	180	12.552	2
2	1	3	5	180	14.644	2
2	1	3	30	180	14.644	2
2	1	9	13	180	12.552	2
2	1	9	26	180	12.552	2
2	4	6	5	180	14.644	2
2	4	6	36	180	14.644	2
3	1	2	4	180	14.644	2
3	1	2	16	180	14.644	2
3	1	9	13	180	12.552	2
3	1	9	26	180	12.552	2
3	5	6	4	180	14.644	2
3	5	6	36	180	14.644	2
4	2	1	9	180	14.644	2
4	2	16	32	180	-0.8786	2
4	2	16	32	0	0.8201	3
4	2	16	33	180	-0.8786	2
4	2	16	33	0	0.8201	3
4	2	16	34	180	-0.8786	2
4	2	16	34	0	0.8201	3
4	6	5	35	180	14.644	2

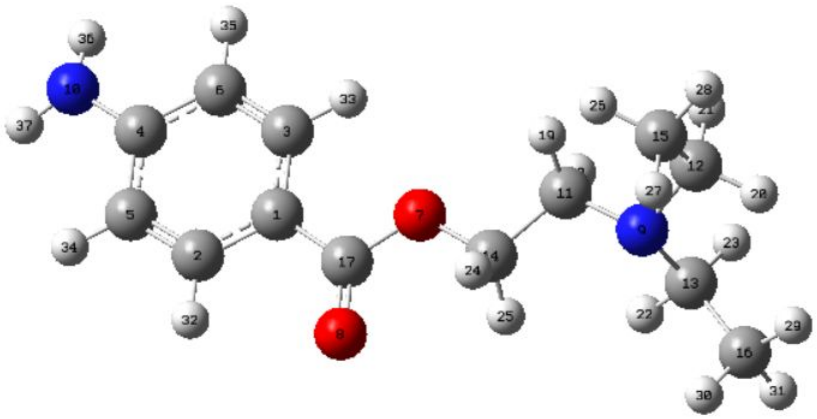
5	3	1	9	180	14.644	2
5	6	4	31	180	14.644	2
6	4	2	16	180	14.644	2
6	5	3	30	180	14.644	2
7	13	9	26	0	3.0041	1
7	13	9	26	180	10.4056	2
7	13	9	26	0	-0.9498	3
7	13	10	8	180	0.8368	2
7	13	10	8	0	0.8368	3
7	13	10	14	0	1.7238	1
7	13	10	14	180	0.2929	2
7	13	10	14	0	0.682	3
7	13	10	17	0	1.3807	1
7	13	10	17	180	-2.9455	2
7	13	10	17	0	0.6443	3
8	10	13	9	180	0.8368	2
8	10	13	9	0	0.6276	3
8	10	14	23	0	-1.5564	1
8	10	14	23	180	-2.5815	2
8	10	14	23	0	0.7071	3
8	10	14	24	0	-1.5564	1
8	10	14	24	180	-2.5815	2
8	10	14	24	0	0.7071	3
8	10	14	25	0	-1.5564	1
8	10	14	25	180	-2.5815	2
8	10	14	25	0	0.7071	3
8	11	12	15	0	-2.9706	1
8	11	12	15	180	-0.1925	2
8	11	12	15	0	2.3012	3
8	11	12	21	0	-1.5564	1
8	11	12	21	180	-2.5815	2
8	11	12	21	0	0.7071	3
8	11	12	22	0	-1.5564	1
8	11	12	22	180	-2.5815	2
8	11	12	22	0	0.7071	3
9	1	2	16	180	14.644	2
9	1	3	30	180	14.644	2
9	13	10	14	0	-1.9414	1
9	13	10	14	180	2.3263	2
9	13	10	14	0	2.9037	3
9	13	10	17	0	-0.8619	1
9	13	10	17	180	1.4477	2
9	13	10	17	0	0.1799	3
10	8	11	12	0	-0.9205	1
10	8	11	12	180	1.6443	2
10	8	11	12	0	0.569	3
10	8	11	18	0	0.8242	1
10	8	11	18	180	-0.8075	2
10	8	11	18	0	1.1757	3
10	8	11	19	0	0.8242	1
10	8	11	19	180	-0.8075	2
10	8	11	19	0	1.1757	3
10	13	9	26	0	-0.615	1
10	13	9	26	180	12.142	2
10	13	9	26	0	2.8075	3
11	8	10	13	180	-0.6276	2
11	8	10	13	0	1.046	3

11	8	10	14	0	-0.9205	1
11	8	10	14	180	1.6443	2
11	8	10	14	0	0.569	3
11	8	10	17	0	0.8242	1
11	8	10	17	180	-0.8075	2
11	8	10	17	0	1.1757	3
11	12	15	27	0	1.3389	1
11	12	15	27	180	-1.318	2
11	12	15	27	0	0.5523	3
11	12	15	28	0	1.3389	1
11	12	15	28	180	-1.318	2
11	12	15	28	0	0.5523	3
11	12	15	29	0	1.3389	1
11	12	15	29	180	-1.318	2
11	12	15	29	0	0.5523	3
12	11	8	20	0	-0.8954	1
12	11	8	20	180	0.6778	2
12	11	8	20	0	0.5858	3
13	10	8	20	180	-0.6276	2
13	10	8	20	0	1.046	3
13	10	14	23	0	-0.5356	1
13	10	14	23	180	0.1213	2
13	10	14	24	0	-0.5356	1
13	10	14	24	180	0.1213	2
13	10	14	25	0	-0.5356	1
13	10	14	25	180	0.1213	2
14	10	8	20	0	-0.8954	1
14	10	8	20	180	0.6778	2
14	10	8	20	0	0.5858	3
15	12	11	18	0	1.3389	1
15	12	11	18	180	-1.318	2
15	12	11	18	0	0.5523	3
15	12	11	19	0	1.3389	1
15	12	11	19	180	-1.318	2
15	12	11	19	0	0.5523	3
16	2	4	31	180	14.644	2
17	10	8	20	0	-0.318	1
17	10	8	20	180	-0.9205	2
17	10	8	20	0	0.7448	3
17	10	14	23	0	0.5941	1
17	10	14	23	180	-2.8995	2
17	10	14	23	0	0.6569	3
17	10	14	24	0	0.5941	1
17	10	14	24	180	-2.8995	2
17	10	14	24	0	0.6569	3
17	10	14	25	0	0.5941	1
17	10	14	25	180	-2.8995	2
17	10	14	25	0	0.6569	3
18	11	8	20	0	-0.318	1
18	11	8	20	180	-0.9205	2
18	11	8	20	0	0.7448	3
18	11	12	21	0	0.5941	1
18	11	12	21	180	-2.8995	2
18	11	12	21	0	0.6569	3
18	11	12	22	0	0.5941	1
18	11	12	22	180	-2.8995	2
18	11	12	22	0	0.6569	3

19	11	8	20	0	-0.318	1
19	11	8	20	180	-0.9205	2
19	11	8	20	0	0.7448	3
19	11	12	21	0	0.5941	1
19	11	12	21	180	-2.8995	2
19	11	12	21	0	0.6569	3
19	11	12	22	0	0.5941	1
19	11	12	22	180	-2.8995	2
19	11	12	22	0	0.6569	3
21	12	15	27	0	0.5941	1
21	12	15	27	180	-2.8995	2
21	12	15	27	0	0.6569	3
21	12	15	28	0	0.5941	1
21	12	15	28	180	-2.8995	2
21	12	15	28	0	0.6569	3
21	12	15	29	0	0.5941	1
21	12	15	29	180	-2.8995	2
21	12	15	29	0	0.6569	3
22	12	15	27	0	0.5941	1
22	12	15	27	180	-2.8995	2
22	12	15	27	0	0.6569	3
22	12	15	28	0	0.5941	1
22	12	15	28	180	-2.8995	2
22	12	15	28	0	0.6569	3
22	12	15	29	0	0.5941	1
22	12	15	29	180	-2.8995	2
22	12	15	29	0	0.6569	3
30	3	5	35	180	14.644	2
31	4	6	36	180	14.644	2
35	5	6	36	180	14.644	2

Improper

Atom Numbers				**φ_0 / deg**	**k_ϕ / kJ mol^{-1} rad^{-2}**
1	2	9	3	0	21.079
2	4	1	16	0	24.0915
3	5	1	30	0	9.0291
4	6	2	31	0	9.0291
9	13	1	26	0	-12.0416
13	10	9	7	0	77.6885
10	8	13	14	0	0
10	8	13	17	0	0
8	11	10	20	0	0
11	12	8	18	0	0
11	12	8	19	0	0
12	15	11	21	0	0
12	15	11	22	0	0
14	23	10	24	0	0
14	23	10	25	0	0
15	27	12	28	0	0
15	27	12	29	0	0
16	32	2	33	0	0
16	32	2	34	0	0
5	6	3	35	0	9.0291
6	5	4	36	0	9.0291



Pc

Atoms

q	σ_{ii} / Å	ε_{ii}/ kJ mol^{-1}	#
-0.181977	3.55005	0.29288	1
-0.100248	3.55005	0.29288	2
-0.089835	3.55005	0.29288	3
0.443268	3.55005	0.29288	4
-0.303764	3.55005	0.29288	5
-0.305537	3.55005	0.29288	6
-0.475574	3.15378	0.63639	7
-0.607795	3.02905	0.50208	8
-0.651129	3.29632	0.83680	9
-0.820874	3.29632	0.83680	10
0.226814	3.87541	0.23012	11
0.428882	3.87541	0.23012	12
0.316206	3.87541	0.23012	13
0.037302	3.87541	0.23012	14
-0.475525	3.87541	0.23012	15
-0.437687	3.87541	0.23012	16
0.838785	3.56359	0.46024	17
-0.010981	2.35197	0.09205	18
0.054276	2.35197	0.09205	19
0.002724	2.35197	0.09205	20
-0.063700	2.35197	0.09205	21
0.026569	2.35197	0.09205	22
-0.038100	2.35197	0.09205	23
0.085672	2.35197	0.09205	24
0.101993	2.35197	0.09205	25
0.129074	2.35197	0.09205	26
0.123994	2.35197	0.09205	27
0.096062	2.35197	0.09205	28
0.128474	2.35197	0.09205	29
0.113177	2.35197	0.09205	30
0.095453	2.35197	0.09205	31
0.149335	2.35197	0.09205	32
0.125368	2.35197	0.09205	33
0.168994	2.35197	0.09205	34
0.169443	2.35197	0.09205	35
0.349489	0.40001	0.19246	36
0.351371	0.40001	0.19246	37

Bonds

Atom Numbers		r_{eq} /Å	k_r/ kJ mol^{-1} Å^{-2}
27	15	1.093	1435.0745
26	15	1.093	1435.0745
24	14	1.093	1435.0745
28	15	1.093	1435.0745
15	12	1.508	1282.1115
32	2	1.084	1597.6730
8	17	1.222	3899.3330
34	5	1.084	1597.6730
2	5	1.374	1678.0685
2	1	1.374	1678.0685
17	1	1.457	1351.3690
17	7	1.355	1746.7195
5	4	1.374	1678.0685
14	7	1.418	1519.6875
14	25	1.093	1435.0745
14	11	1.508	1282.1115
1	3	1.374	1678.0685
30	16	1.093	1435.0745
19	11	1.093	1435.0745
12	9	1.451	1530.8250
12	20	1.093	1435.0745
12	21	1.093	1435.0745
9	11	1.451	1530.8250
9	13	1.451	1530.8250
4	10	1.398	1857.2275
4	6	1.374	1678.0685
11	18	1.093	1435.0745
37	10	1.018	1980.0780
29	16	1.093	1435.0745
3	6	1.374	1678.0685
3	33	1.084	1597.6730
10	36	1.018	1980.0780
16	13	1.508	1282.1115
16	31	1.093	1435.0745
6	35	1.084	1597.6730
13	22	1.093	1435.0745
13	23	1.093	1435.0745

Angles

Atom Numbers			θ_{eq} / deg	k_θ / kJ mol^{-1} rad^{-2}
2	1	3	119.977	402.88
2	1	17	114.475	480.57
3	1	17	114.475	480.57
1	2	5	119.977	402.88
1	2	32	120.571	339.05
5	2	32	120.571	339.05
1	3	6	119.977	402.88
1	3	33	120.571	339.05
6	3	33	120.571	339.05
5	4	6	119.977	402.88
5	4	10	121.633	629.31
6	4	10	121.633	629.31
2	5	4	119.977	402.88
2	5	34	120.571	339.05
4	5	34	120.571	339.05

3	6	4	119.977	402.88
3	6	35	120.571	339.05
4	6	35	120.571	339.05
14	7	17	108.055	555.84
11	9	12	107.018	656.41
11	9	13	107.018	656.41
12	9	13	107.018	656.41
4	10	36	110.288	398.66
4	10	37	110.288	398.66
36	10	37	109.160	337.24
9	11	14	108.290	467.91
9	11	18	110.297	393.25
9	11	19	110.297	393.25
14	11	18	110.549	383.00
14	11	19	110.549	383.00
18	11	19	108.836	310.74
9	12	15	108.290	467.91
9	12	20	110.297	393.25
9	12	21	110.297	393.25
15	12	20	110.549	383.00
15	12	21	110.549	383.00
20	12	21	108.836	310.74
9	13	16	108.290	467.91
9	13	22	110.297	393.25
9	13	23	110.297	393.25
16	13	22	110.549	383.00
16	13	23	110.549	383.00
22	13	23	108.836	310.74
7	14	11	108.133	597.39
7	14	24	108.577	470.32
7	14	25	108.577	470.32
11	14	24	110.549	383.00
11	14	25	110.549	383.00
24	14	25	108.836	310.74
12	15	26	110.549	383.00
12	15	27	110.549	383.00
12	15	28	110.549	383.00
26	15	27	108.836	310.74
26	15	28	108.836	310.74
27	15	28	108.836	310.74
13	16	29	110.549	383.00
13	16	30	110.549	383.00
13	16	31	110.549	383.00
29	16	30	108.836	310.74
29	16	31	108.836	310.74
30	16	31	108.836	310.74
1	17	7	102.881	486.58
1	17	8	119.968	442.02
7	17	8	124.425	695.55

Dihedrals

Atom Numbers				**δ / deg**	**k_ϕ / kJ mol^{-1}**	**m**
1	2	5	4	180	14.644	2
1	2	5	34	180	14.644	2
1	3	6	4	180	14.644	2
1	3	6	35	180	14.644	2
1	17	7	14	180	11.506	2

2	1	3	6	180	14.644	2
2	1	3	33	180	14.644	2
2	1	17	7	180	5.23	2
2	1	17	8	180	5.23	2
2	5	4	6	180	14.644	2
2	5	4	10	180	14.644	2
3	1	2	5	180	14.644	2
3	1	2	32	180	14.644	2
3	1	17	7	180	5.23	2
3	1	17	8	180	5.23	2
3	6	4	5	180	14.644	2
3	6	4	10	180	14.644	2
4	5	2	32	180	14.644	2
4	6	3	33	180	14.644	2
5	2	1	17	180	14.644	2
5	4	6	35	180	14.644	2
5	4	10	36	0	1.4937	1
5	4	10	36	180	5.4978	2
5	4	10	36	0	7.0166	3
5	4	10	37	0	1.4937	1
5	4	10	37	180	5.4978	2
5	4	10	37	0	7.0166	3
6	3	1	17	180	14.644	2
6	4	5	34	180	14.644	2
6	4	10	36	0	1.4937	1
6	4	10	36	180	5.4978	2
6	4	10	36	0	7.0166	3
6	4	10	37	0	1.4937	1
6	4	10	37	180	5.4978	2
6	4	10	37	0	7.0166	3
7	14	11	9	0	0.6276	3
7	14	11	18	0	-1.3682	1
7	14	11	18	180	2.2426	2
7	14	11	18	0	0.5858	3
7	14	11	19	0	-1.3682	1
7	14	11	19	180	2.2426	2
7	14	11	19	0	0.5858	3
8	17	7	14	0	1.4267	1
8	17	7	14	180	15.0289	2
8	17	7	14	0	-1.9581	3
9	11	14	24	0	-1.5564	1
9	11	14	24	180	-2.5815	2
9	11	14	24	0	0.7071	3
9	11	14	25	0	-1.5564	1
9	11	14	25	180	-2.5815	2
9	11	14	25	0	0.7071	3
9	12	15	26	0	-1.5564	1
9	12	15	26	180	-2.5815	2
9	12	15	26	0	0.7071	3
9	12	15	27	0	-1.5564	1
9	12	15	27	180	-2.5815	2
9	12	15	27	0	0.7071	3
9	12	15	28	0	-1.5564	1
9	12	15	28	180	-2.5815	2
9	12	15	28	0	0.7071	3
9	13	16	29	0	-1.5564	1
9	13	16	29	180	-2.5815	2

9	13	16	29	0	0.7071	3
9	13	16	30	0	-1.5564	1
9	13	16	30	180	-2.5815	2
9	13	16	30	0	0.7071	3
9	13	16	31	0	-1.5564	1
9	13	16	31	180	-2.5815	2
9	13	16	31	0	0.7071	3
10	4	5	34	180	14.644	2
10	4	6	35	180	14.644	2
11	9	12	15	0	-0.9205	1
11	9	12	15	180	1.6443	2
11	9	12	15	0	0.569	3
11	9	12	20	0	0.8242	1
11	9	12	20	180	-0.8075	2
11	9	12	20	0	1.1757	3
11	9	12	21	0	0.8242	1
11	9	12	21	180	-0.8075	2
11	9	12	21	0	1.1757	3
11	9	13	16	0	-0.9205	1
11	9	13	16	180	1.6443	2
11	9	13	16	0	0.569	3
11	9	13	22	0	0.8242	1
11	9	13	22	180	-0.8075	2
11	9	13	22	0	1.1757	3
11	9	13	23	0	0.8242	1
11	9	13	23	180	-0.8075	2
11	9	13	23	0	1.1757	3
11	14	7	17	0	-1.1464	1
11	14	7	17	0	0.6694	3
12	9	11	14	0	-0.9205	1
12	9	11	14	180	1.6443	2
12	9	11	14	0	0.569	3
12	9	11	18	0	0.8242	1
12	9	11	18	180	-0.8075	2
12	9	11	18	0	1.1757	3
12	9	11	19	0	0.8242	1
12	9	11	19	180	-0.8075	2
12	9	11	19	0	1.1757	3
12	9	13	16	0	-0.9205	1
12	9	13	16	180	1.6443	2
12	9	13	16	0	0.569	3
12	9	13	22	0	0.8242	1
12	9	13	22	180	-0.8075	2
12	9	13	22	0	1.1757	3
12	9	13	23	0	0.8242	1
12	9	13	23	180	-0.8075	2
12	9	13	23	0	1.1757	3
13	9	11	14	0	-0.9205	1
13	9	11	14	180	1.6443	2
13	9	11	14	0	0.569	3
13	9	11	18	0	0.8242	1
13	9	11	18	180	-0.8075	2
13	9	11	18	0	1.1757	3
13	9	11	19	0	0.8242	1
13	9	11	19	180	-0.8075	2
13	9	11	19	0	1.1757	3
13	9	12	15	0	-0.9205	1

13	9	12	15	180	1.6443	2
13	9	12	15	0	0.569	3
13	9	12	20	0	0.8242	1
13	9	12	20	180	-0.8075	2
13	9	12	20	0	1.1757	3
13	9	12	21	0	0.8242	1
13	9	12	21	180	-0.8075	2
13	9	12	21	0	1.1757	3
17	1	2	32	180	4.184	2
17	1	3	33	180	4.184	2
17	7	14	24	0	1.1966	1
17	7	14	24	0	-0.636	3
17	7	14	25	0	1.1966	1
17	7	14	25	0	-0.636	3
18	11	14	24	0	0.5941	1
18	11	14	24	180	-2.8995	2
18	11	14	24	0	0.6569	3
18	11	14	25	0	0.5941	1
18	11	14	25	180	-2.8995	2
18	11	14	25	0	0.6569	3
19	11	14	24	0	0.5941	1
19	11	14	24	180	-2.8995	2
19	11	14	24	0	0.6569	3
19	11	14	25	0	0.5941	1
19	11	14	25	180	-2.8995	2
19	11	14	25	0	0.6569	3
20	12	15	26	0	0.5941	1
20	12	15	26	180	-2.8995	2
20	12	15	26	0	0.6569	3
20	12	15	27	0	0.5941	1
20	12	15	27	180	-2.8995	2
20	12	15	27	0	0.6569	3
20	12	15	28	0	0.5941	1
20	12	15	28	180	-2.8995	2
20	12	15	28	0	0.6569	3
21	12	15	26	0	0.5941	1
21	12	15	26	180	-2.8995	2
21	12	15	26	0	0.6569	3
21	12	15	27	0	0.5941	1
21	12	15	27	180	-2.8995	2
21	12	15	27	0	0.6569	3
21	12	15	28	0	0.5941	1
21	12	15	28	180	-2.8995	2
21	12	15	28	0	0.6569	3
22	13	16	29	0	0.5941	1
22	13	16	29	180	-2.8995	2
22	13	16	29	0	0.6569	3
22	13	16	30	0	0.5941	1
22	13	16	30	180	-2.8995	2
22	13	16	30	0	0.6569	3
22	13	16	31	0	0.5941	1
22	13	16	31	180	-2.8995	2
22	13	16	31	0	0.6569	3
23	13	16	29	0	0.5941	1
23	13	16	29	180	-2.8995	2
23	13	16	29	0	0.6569	3
23	13	16	30	0	0.5941	1

23	13	16	30	180	-2.8995	2
23	13	16	30	0	0.6569	3
23	13	16	31	0	0.5941	1
23	13	16	31	180	-2.8995	2
23	13	16	31	0	0.6569	3
32	2	5	34	180	14.644	2
33	3	6	35	180	14.644	2

Improper

Atom Numbers				**φ_0 / deg**	**k_ϕ / kJ mol^{-1} rad^{-2}**
1	3	17	2	0	16.259
2	5	1	32	0	9.0291
5	4	2	34	0	9.0291
4	10	5	6	0	27.6981
17	7	1	8	0	76.4835
14	11	7	24	0	0
14	24	7	25	0	0
11	9	14	19	0	0
11	19	14	18	0	0
9	12	11	13	0	0
12	15	9	20	0	0
12	15	9	21	0	0
13	16	9	22	0	0
13	16	9	23	0	0
15	27	12	26	0	0
15	27	12	28	0	0
16	30	13	29	0	0
16	30	13	31	0	0
3	6	1	33	0	9.0291
6	3	4	35	0	9.0291
10	37	4	36	0	2.41

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

		c / g mL^{-1}				
$N_{\text{ArOa 1:1}}$	N_{ANS}	Bp	Pl	Pc	*T* / K	*P* / bar
500	0	0	0	0	298	1
500	56	0.17	0.13	0.14	298	1
500	125	0.37	0.28	0.30	298	1
500	214	0.63	0.48	0.52	298	1
500	333	0.99	0.75	0.81	298	1
500	500	1.48	1.13	1.21	298	1

Table S3. Atoms-in-a-molecule analysis of the reported ArGa_Bp, ArGa_Pc and ArGa_Pl systems calculated at B3LYP/6-311++g(d,p) level. Bond critical point (BCP, (3,-1)) are given, electron density (ρ) and laplacian of electron density ($\nabla^2\rho$) at the corresponding BCP are provided as a guide for AIM and RDG analysis.

Structure	BCP	ρ / a.u.	$\nabla^2\rho$ / a.u.
ArGa_Bp	111	-6.6E-03	1.4E-01
	117	-2.4E-03	1.3E-01
	159	5.2E-04	1.3E-02
	173	1.3E-03	3.5E-02
	176	3.9E-04	1.3E-02
	185	1.2E-03	4.3E-02
ArGa_Pc	102	9.6E-04	2.6E-02
	103	1.9E-03	4.7E-02
	104	-4.2E-03	1.3E-01
	106	7.5E-05	8.0E-04
	111	-5.0E-03	1.4E-01
	112	4.3E-04	7.4E-03
ArGa_Pl	98	4.4E-04	9.1E-03
	99	3.3E-04	4.4E-03
	113	-8.4E-03	1.4E-01
	119	-1.7E-03	1.2E-01
	122	5.3E-04	1.4E-02
	151	1.3E-03	2.6E-02
	155	9.0E-04	2.6E-02
	156	1.2E-03	3.4E-02
	159	1.2E-03	2.6E-02
	176	5.8E-04	1.1E-02

Table S4. Atoms-in-a-molecule analysis of the reported ArOa_Bp, ArOa_Pc and ArOa_Pl systems calculated at B3LYP/6-311++g(d,p) level. Bond critical point (BCP, (3,-1)) are given, electron density (ρ) and laplacian of electron density ($\nabla^2\rho$) at the corresponding BCP are provided as a guide for AIM and RDG analysis.

Structure	BCP	ρ / a.u.	$\nabla^2\rho$ / a.u.
ArOa_Bp	90	4.2E-04	7.2E-03
	126	5.4E-04	1.2E-02
	128	1.9E-03	4.1E-02
	136	1.1E-03	3.6E-02
	141	-2.6E-03	1.3E-01
	148	5.4E-04	1.7E-02
	156	4.8E-04	1.0E-02
	157	-4.6E-03	1.5E-01
	175	-2.7E-01	9.1E-01
	180	6.1E-04	1.5E-02
ArOa_Pc	109	7.0E-05	1.3E-01
	113	1.1E-03	3.5E-02
	117	9.7E-04	2.9E-02
	118	8.5E-04	2.0E-02
	119	5.9E-04	1.6E-02
	123	-4.1E-03	1.5E-01
	142	1.1E-03	3.4E-02
	146	5.9E-04	1.5E-02
ArOa_Pl	94	5.3E-04	1.3E-01
	100	6.3E-04	1.7E-02
	101	2.0E-03	5.6E-02
	114	6.4E-04	1.7E-02
	123	1.7E-03	5.0E-02

Table S5. Atoms-in-a-molecule analysis of the reported ArTa_Bp, ArTa_Pc and ArTa_Pl systems calculated at B3LYP/6-311++g(d,p) level. Bond critical point (BCP, (3,-1)) are given, electron density (ρ) and laplacian of electron density ($\nabla^2\rho$) at the corresponding BCP are provided as a guide for AIM and RDG analysis.

Structure	BCP	ρ / a.u.	$\nabla^2\rho$ / a.u.
ArTa_Bp	105	-9.0E-03	9.5E-02
	114	2.6E-03	1.0E-01
	117	3.6E-04	1.1E-02
	125	5.3E-04	1.2E-02
	137	1.6E-04	1.7E-03
	139	3.9E-04	8.4E-03
	143	4.9E-04	8.7E-03
	157	9.6E-04	1.8E-02
	159	1.0E-03	3.3E-02
	162	7.5E-04	1.7E-02
	167	5.3E-04	1.1E-02
	168	2.0E-03	4.4E-02
	205	4.0E-04	7.3E-03
ArTa_Pc	102	3.1E-03	1.0E-01
	106	2.0E-03	4.1E-02
	122	5.8E-04	1.2E-02
	125	2.8E-03	7.2E-02
	127	6.7E-04	1.5E-02
	130	1.4E-03	3.0E-02
	134	2.1E-03	5.1E-02
	135	4.6E-04	1.5E-02
ArTa_Pl	89	4.4E-04	1.4E-02
	94	2.5E-03	5.5E-02
	98	1.3E-03	4.1E-02
	106	1.0E-03	2.9E-02
	108	4.2E-04	7.5E-03
	116	6.3E-04	1.4E-02
	124	1.0E-03	2.7E-02
	125	2.2E-03	6.5E-02
	139	6.8E-04	1.2E-02
	142	3.9E-04	1.3E-02
	144	7.2E-04	1.5E-02

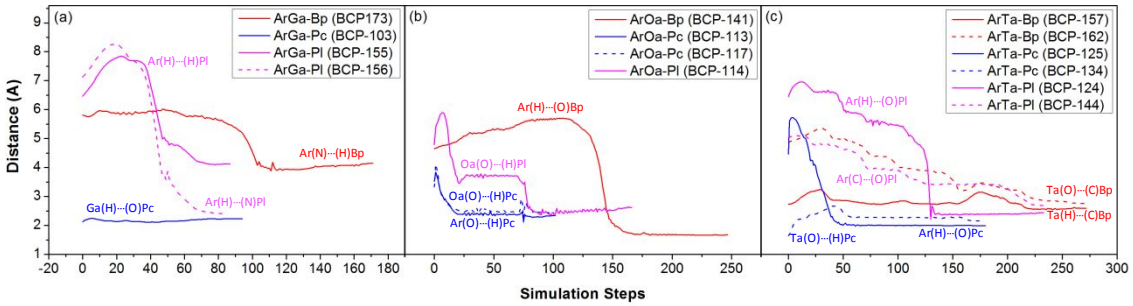


Figure S1. Distance evolution between BCP forming atoms throughout the geometry optimization simulations, which are extracted from trajectory files.

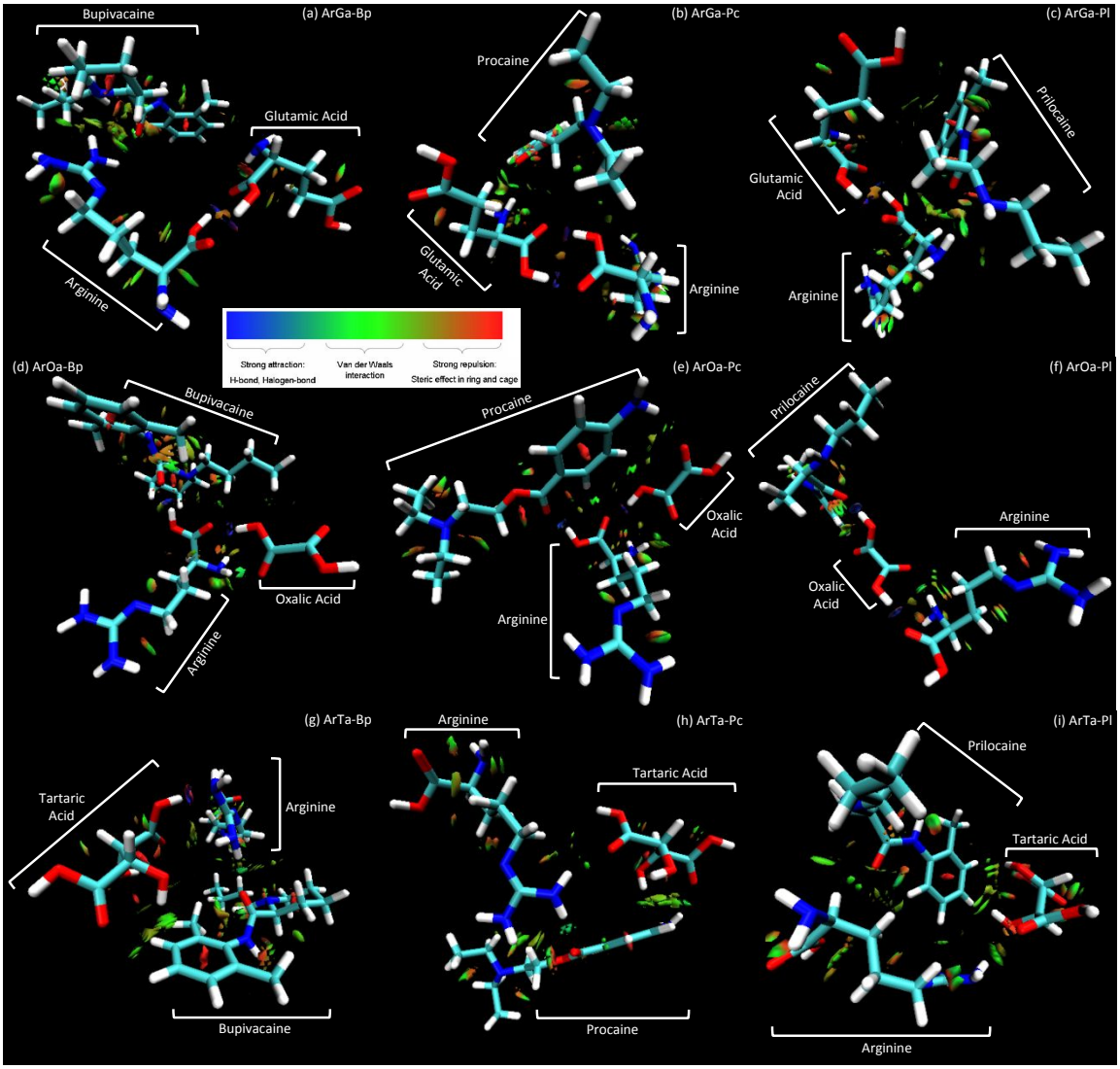


Figure S2. Reduced density gradient (RDG) iso-surfaces (green or green-brown color indicates van der Waals interactions) are shown for: (a) ArGa-Bp, (b) ArGa-Pc, (c) ArGa-Pl, (d) ArOa-Bp, (e) ArOa-Pc, (f) ArOa-Pl, (g) ArTa-Bp, (h) ArTa-Pc, (i) ArTa-Pl.

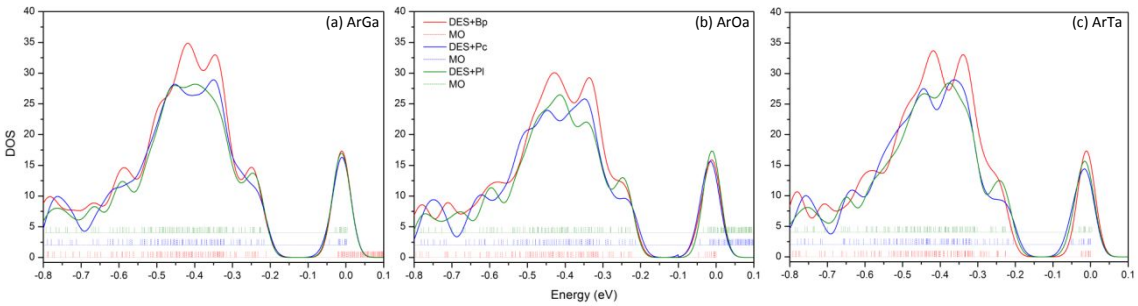


Figure S3. Density of states (DOS) as a function of orbital energy, E, for ArGa, ArOa and ArTa structures interacting with studied APIs. Discrete vertical lines close to the x-axis correspond to the molecular orbitals (MO) for each structure.

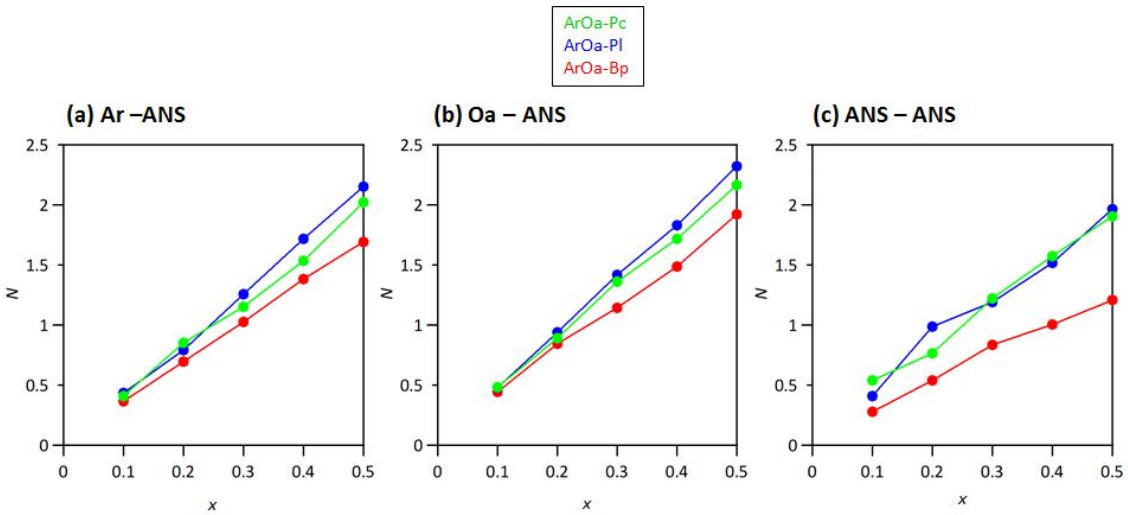


Figure S4. Solvation numbers, *N*, around a central ANS (Bp, Pl or PC) molecule obtained from the integration of the corresponding center-of-mass radial distribution functions (r = 7.5 Å) for the reported ArOa + ANS (Bp, Pl or Pc) solutions (x stands for ANS mole fraction) from MD simulations at 298 K and 1 bar.

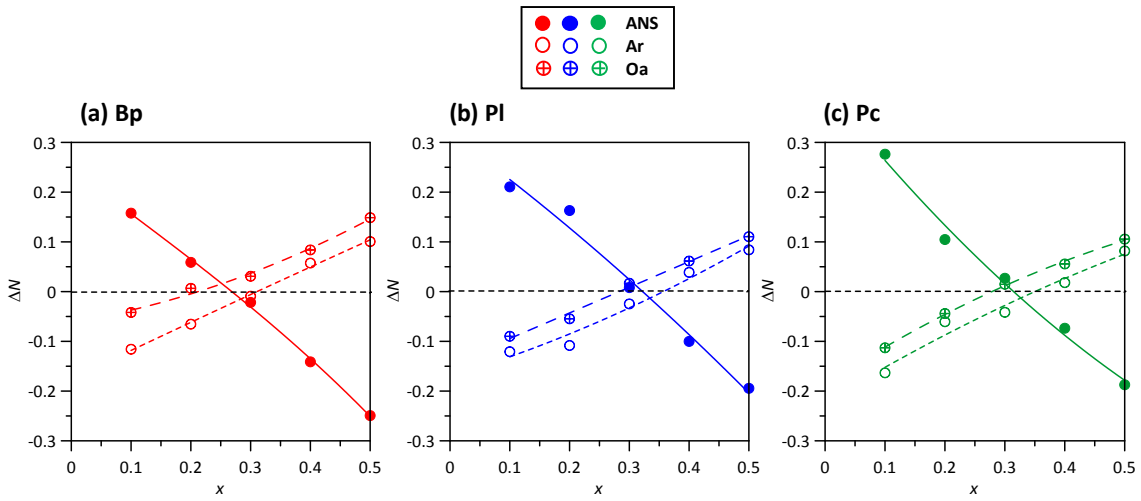


Figure S5. Excess solvation number, Δ*N*, around central ANS molecule calculated from *N* reported in Figure 9 for ArOa + ANS (Bp, Pl or Pc) solutions (x stands for ANS mole fraction) from MD simulations at 298 K and 1 bar.

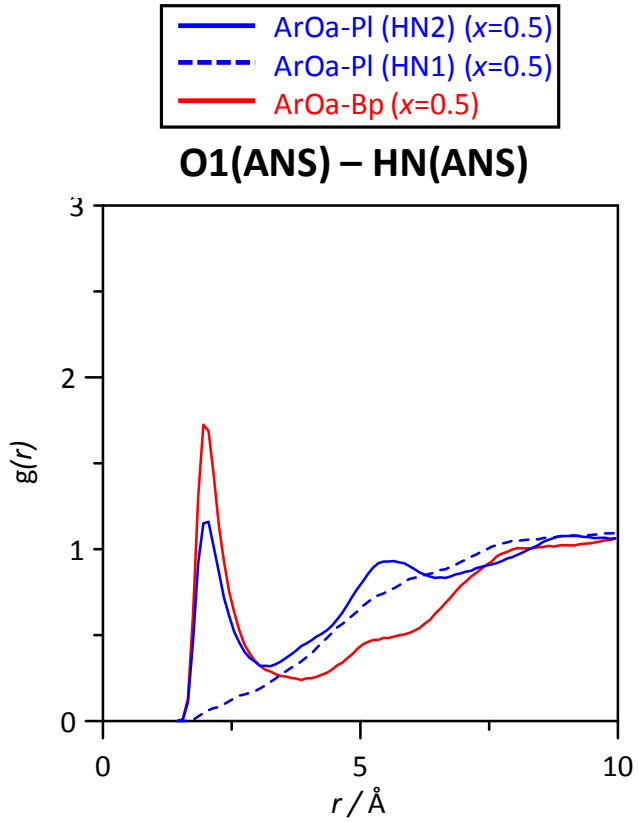


Figure S6. Site-site (atomic labels as in Figure 1) radial distribution functions, $g(r)$, for the reported ArOa + ANS (Bp, Pl or Pc) solutions (x stands for ANS mole fraction) from MD simulations at 298 K and 1 bar. Results in this Figure show ANS – ANS interactions.

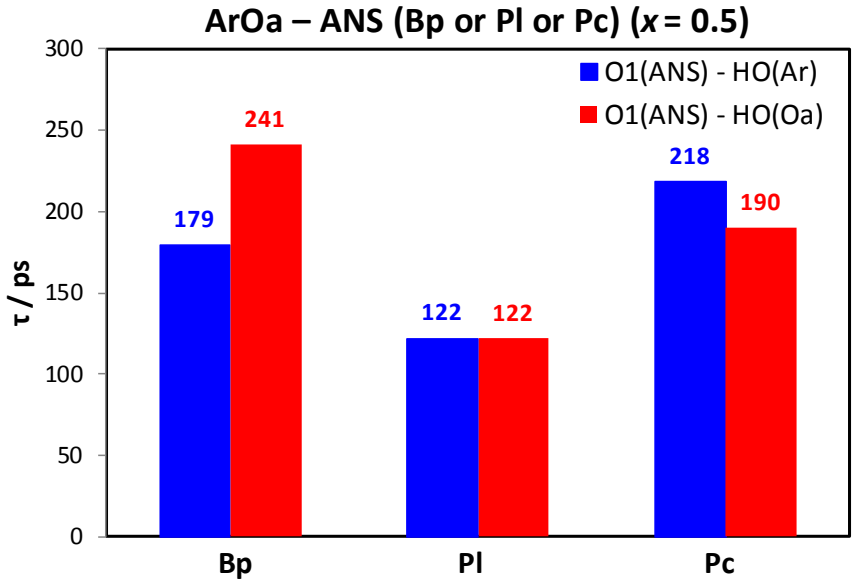


Figure S7. Residence time, τ, in the first solvation sphere around a central ANS (Bp, Pl or Pc) molecule for the reported atoms in Ar or Oa in ArOa + ANS (Bp, Pl or Pc) solutions (x =0.5, where x stands for ANS mole fraction) from MD simulations at 298 K and 1 bar. Atoms labels as in Figure 1. Solvation spheres were defined with radii r = 2.5 Å, corresponding to the first minima in radial distribution functions reported in Figures 11b and 12b.

References

(1) Gutiérrez, A.; Atilhan, M.; Aparicio, S. Design of Arginine Based Therapeutic Deep Eutectic Solvents as Drug Solubilization Vehicle for Active Pharmaceutical Ingredient. *Phys. Chem. Chem. Phys.* 2019, **21**, 10621-10634.