Choline-Based Ionic Liquids on Graphite Surfaces and Carbon Nanotubes Solvation: a Molecular Dynamics Study

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Supporting Information

Table S1. Forcefield parameters for $[CH]^+$ cation, and $[BE]^-$ and $[SA]^-$ anions

The general form of the applied force field is:

$$E = \sum_{bonds} k_r (r - r_{eq})^2 + \sum_{angles} k_\theta (\theta - \theta_{eq})^2 + \\ + \sum_{torsions} k_\phi (1 + \cos(m\phi - \delta))$$

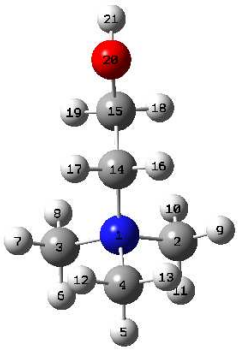
$$+ \sum_i \sum_j \left\{ 4\varepsilon_{ij} \left[\left(\frac{\sigma_{ij}}{r_{ij}} \right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}} \right)^{6} \right] + \frac{q_i q_j e^2}{4\pi\varepsilon_0 r_{ij}} \right\}$$

Dihedrals for $[BE]^-$ and $[SAL]^-$ were described according to:

$$E_{torsional} = \sum_{torsions} \frac{k_{\phi,1}}{2}\left[1 + \cos(\phi)\right] + \frac{k_{\phi,2}}{2}\left[1 - \cos(2\phi)\right] + \frac{k_{\phi,3}}{2}\left[1 + \cos(3\phi)\right]$$

Improper dihedrals were described according to:

$E_{improper} = k_{\square}(\square - \square_0)^2$



$[CH]^+$

Atom Type	*q*	σ_{ii} / Å	ε_{ii} /kJ mol^{-1}	*Numbering*
N1	0.1120	3.1000	0.8370	1
C1	-0.2450	3.4500	0.3350	2
C1	-0.2450	3.4500	0.3350	3
C1	-0.3510	3.4500	0.3350	4
H1	0.1770	2.2100	0.0920	5
H1	0.1490	2.2100	0.0920	6
H1	0.1490	2.2100	0.0920	7
H1	0.1490	2.2100	0.0920	8
H1	0.1490	2.2100	0.0920	9
H1	0.1490	2.2100	0.0920	10
H1	0.1490	2.2100	0.0920	11
H1	0.1770	2.2100	0.0920	12
H1	0.1770	2.2100	0.0920	13
C2	-0.0520	3.6400	0.2300	14
C3	0.3030	3.6400	0.2300	15
H2	0.1270	2.2100	0.0920	16
H2	0.1270	2.2100	0.0920	17
H3	0.0110	0.0000	0.0000	18
H3	0.0110	0.0000	0.0000	19
O1	-0.6970	3.9500	0.6370	20
H4	0.4740	0.0000	0.0000	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

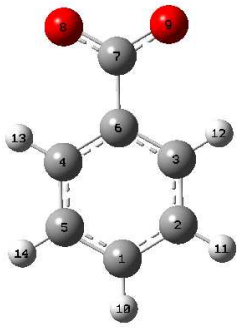
Angles

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



[BE]$^-$

Atom Type	*q*	σ_{ii} / Å	ε_{ii} /kJ mol^{-1}	*Numbering*
C8	−0.13100	3.33000	0.307524	1
C7	−0.11300	3.33000	0.307524	2
C6	−0.09500	3.33000	0.307524	3
C6	−0.09500	3.33000	0.307524	4
C7	−0.11300	3.33000	0.307524	5
C5	0.00200	3.33000	0.307524	6
C4	0.81800	3.52000	0.461286	7
O2	−0.79900	2.80000	0.834708	8
O2	−0.79900	2.80000	0.834708	9
H7	0.05900	2.28000	0.131796	10
H6	0.05200	2.28000	0.131796	11
H5	0.08100	2.28000	0.131796	12
H5	0.08100	2.28000	0.131796	13
H6	0.05200	2.28000	0.131796	14

Bonds

Atom Numbers		r_{eq} /Å	k_r / kJ mol^{-1} Å^{-2}
1	5	1.40000	1962.29
1	10	1.08000	1535.53
1	2	1.40000	1962.29
2	3	1.40000	1962.29
2	11	1.08000	1535.53
3	12	1.08000	1535.53
3	6	1.40000	1962.29
4	5	1.40000	1962.29
4	13	1.08000	1535.53
4	6	1.40000	1962.29
5	14	1.08000	1535.53
6	7	1.49000	1673.60
7	9	1.27800	1640.12
7	8	1.27800	1640.12

Angles

Atom Numbers			θ_{eq} / deg	k_θ / kJ mol^{-1} rad^{-2}
5	1	10	120.0000	146.44
5	1	2	120.0000	263.59
10	1	2	120.0000	146.44
1	2	3	120.0000	263.59
1	2	11	120.0000	146.44
3	2	11	120.0000	146.44
2	3	12	120.0000	146.44
2	3	6	120.0000	263.59
12	3	6	120.0000	146.44
5	4	13	120.0000	146.44
5	4	6	120.0000	263.59

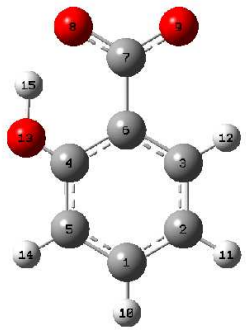
13	4	6	120.0000	146.44
1	5	4	120.0000	263.59
1	5	14	120.0000	146.44
4	5	14	120.0000	146.44
3	6	4	120.0000	263.59
3	6	7	120.0000	355.68
4	6	7	120.0000	355.68
6	7	9	120.0000	336.96
6	7	8	120.0000	336.96
9	7	8	120.0000	347.27

Dihedrals

Atom Numbers				$k_{\phi,1}$ / kJ mol^{-1}	$k_{\phi,2}$ / kJ mol^{-1}	$k_{\phi,3}$ / kJ mol^{-1}
10	1	5	4	0	30.334	0
10	1	5	14	0	30.334	0
2	1	5	4	0	30.334	0
2	1	5	14	0	30.334	0
5	1	2	3	0	30.334	0
5	1	2	11	0	30.334	0
10	1	2	3	0	30.334	0
10	1	2	11	0	30.334	0
1	2	3	12	0	30.334	0
1	2	3	6	0	30.334	0
11	2	3	12	0	30.334	0
11	2	3	6	0	30.334	0
2	3	6	4	0	30.334	0
2	3	6	7	0	30.334	0
12	3	6	4	0	30.334	0
12	3	6	7	0	30.334	0
13	4	5	1	0	30.334	0
13	4	5	14	0	30.334	0
6	4	5	1	0	30.334	0
6	4	5	14	0	30.334	0
5	4	6	3	0	30.334	0
5	4	6	7	0	30.334	0
13	4	6	3	0	30.334	0
13	4	6	7	0	30.334	0
3	6	7	9	0	8.786	0
3	6	7	8	0	8.786	0
4	6	7	9	0	8.786	0
4	6	7	8	0	8.786	0

Improper

Atom Numbers				□$_0$ / deg	k_ϕ / kJ mol^{-1} rad^{-2}
3	6	2	12	0.0000	62.800
2	1	3	11	0.0000	62.800
1	5	2	10	0.0000	62.800
5	4	1	14	0.0000	62.800
4	5	6	13	0.0000	62.800
6	3	4	7	0.0000	62.800
7	6	8	9	0.0000	62.800



[SAL]$^-$

Atom Type	*q*	σ_{ii} / Å	ε_{ii} /kJ mol^{-1}	*Numbering*
C8	−0.04200	3.33000	0.307524	1
C7	−0.22600	3.33000	0.307524	2
C6	−0.01400	3.33000	0.307524	3
C9	0.55400	3.33000	0.307524	4
C10	−0.34000	3.33000	0.307524	5
C5	−0.32800	3.33000	0.307524	6
C4	0.92100	3.52000	0.461286	7
O2	−0.84900	2.80000	0.834708	8
O2	−0.76700	2.80000	0.834708	9
H7	0.05300	2.28000	0.131796	10
H6	0.07000	2.28000	0.131796	11
H5	0.08200	2.28000	0.131796	12
O3	−0.76200	2.89000	0.746844	13
H9	0.13000	2.28000	0.131796	14
H8	0.51800	0.00000	0.000000	15

Bonds

Atom Numbers		r_{eq} /Å	k_r / kJ mol^{-1} Å^{-2}
1	5	1.40000	1962.29
1	10	1.08000	1535.53
1	2	1.40000	1962.29
2	3	1.40000	1962.29
2	11	1.08000	1535.53
3	12	1.08000	1535.53
3	6	1.40000	1962.29
4	5	1.40000	1962.29
4	13	1.36400	1882.80
4	6	1.40000	1962.29
5	14	1.08000	1535.53
6	7	1.49000	1673.60
7	9	1.27800	1640.12
7	8	1.27800	1640.12
13	15	0.94500	2313.75

Angles

Atom Numbers			θ_{eq} / deg	k_θ / kJ mol^{-1} rad^{-2}
5	1	10	120.0000	146.44
5	1	2	120.0000	263.59
10	1	2	120.0000	146.44
1	2	3	120.0000	263.59
1	2	11	120.0000	146.44
3	2	11	120.0000	146.44
2	3	12	120.0000	146.44
2	3	6	120.0000	263.59

12	3	6	120.0000	146.44
5	4	13	120.0000	292.88
5	4	6	120.0000	263.59
13	4	6	120.0000	292.88
1	5	4	120.0000	263.59
1	5	14	120.0000	146.44
4	5	14	120.0000	146.44
3	6	4	120.0000	263.59
3	6	7	120.0000	355.68
4	6	7	120.0000	355.68
6	7	9	120.0000	336.96
6	7	8	120.0000	336.96
9	7	8	120.0000	347.27
4	13	15	113.0000	146.44

Dihedrals

Atom Numbers				$k_{\phi,1}$ / kJ mol^{-1}	$k_{\phi,2}$ / kJ mol^{-1}	$k_{\phi,3}$ / kJ mol^{-1}
10	1	5	4	0	30.334	0
10	1	5	14	0	30.334	0
2	1	5	4	0	30.334	0
2	1	5	14	0	30.334	0
5	1	2	3	0	30.334	0
5	1	2	11	0	30.334	0
10	1	2	3	0	30.334	0
10	1	2	11	0	30.334	0
1	2	3	12	0	30.334	0
1	2	3	6	0	30.334	0
11	2	3	12	0	30.334	0
11	2	3	6	0	30.334	0
2	3	6	4	0	30.334	0
2	3	6	7	0	30.334	0
12	3	6	4	0	30.334	0
12	3	6	7	0	30.334	0
13	4	5	1	0	30.334	0
13	4	5	14	0	30.334	0
6	4	5	1	0	30.334	0
6	4	5	14	0	30.334	0
5	4	6	3	0	30.334	0
5	4	6	7	0	30.334	0
13	4	6	3	0	30.334	0
13	4	6	7	0	30.334	0
3	6	7	9	0	8.786	0
3	6	7	8	0	8.786	0
4	6	7	9	0	8.786	0
4	6	7	8	0	8.786	0
5	4	13	15	0	7.037	0
6	4	13	15	0	7.037	0

Improper

Atom Numbers				□$_0$ / deg	k_ϕ / kJ mol^{-1} rad^{-2}
3	6	2	12	0.0000	62.800
2	1	3	11	0.0000	62.800
1	5	2	10	0.0000	62.800
5	4	1	14	0.0000	62.800
4	5	6	13	0.0000	62.800
6	3	4	7	0.0000	62.800
7	6	8	9	0.0000	62.800