Supporting information

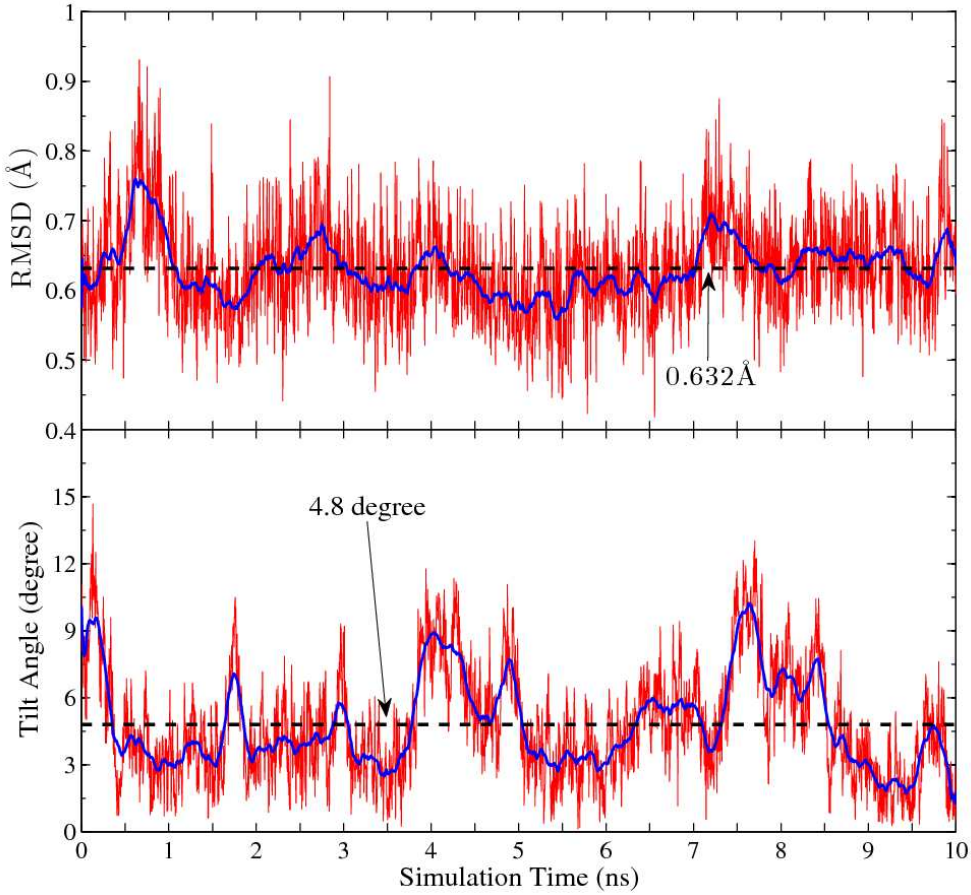

Figure S1. Time profile of RMSD (top) and tilt angle (bottom) in the absence of ions in gA channel.

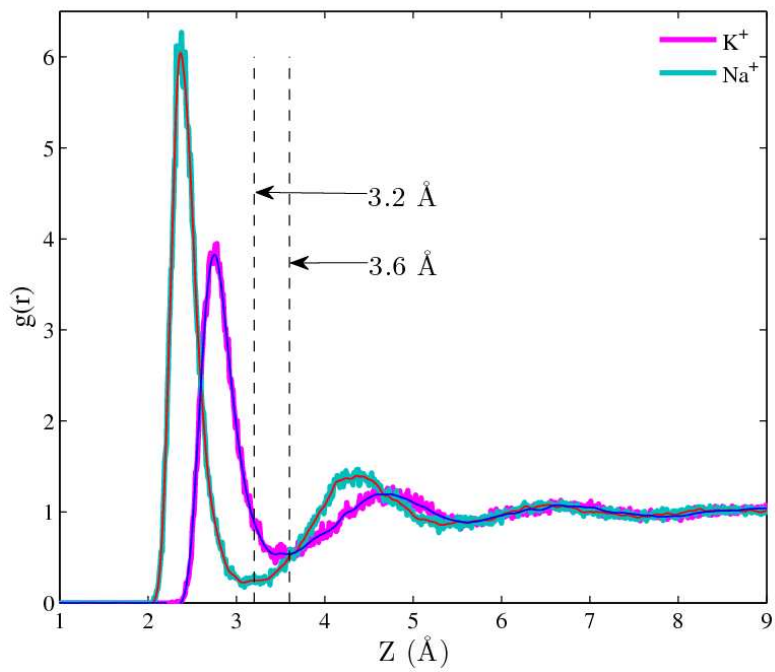

Figure S2. The water oxygen atoms radial distribution functions of K^+ and Na^+ in bulk.

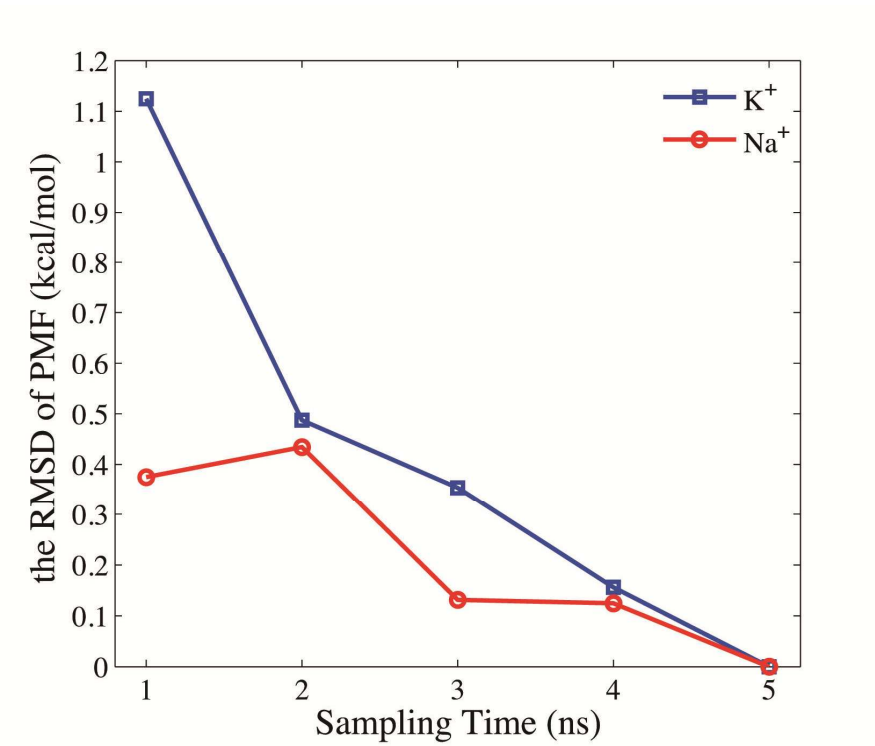

Figure S3. The root mean square deviation of PMFs with different sampling time with respect to 5ns.

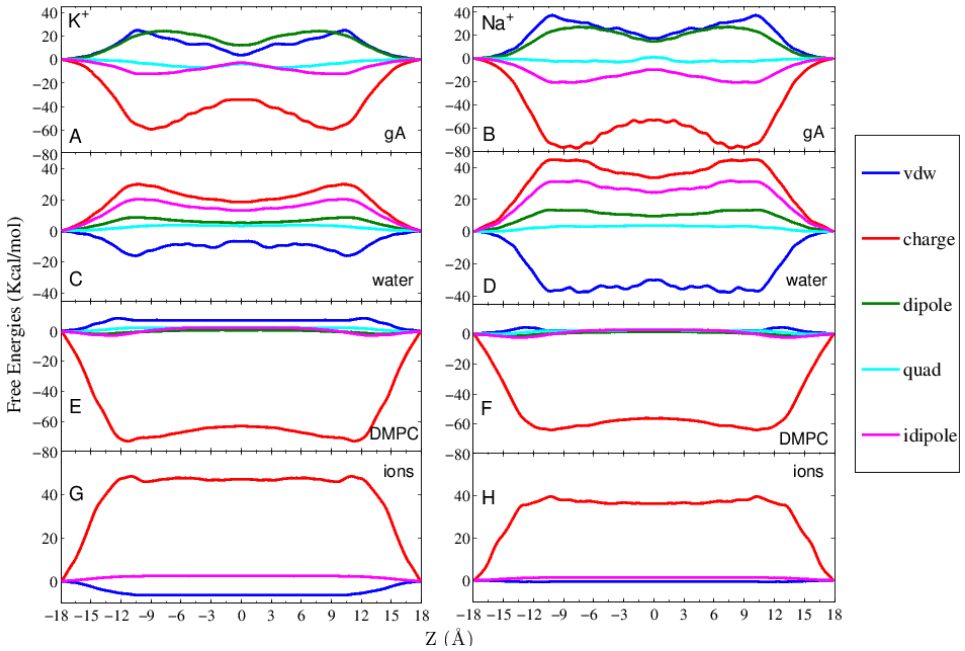

Figure S4. The force component of the PMF contribution from gA (A for K+ and B for Na+), water (C for K+ and D for Na+), DMPC (E for K+ and F for Na+) and ions (H for K+ and I for Na+). The total contribution from each system component are composed of charge, dipole, quadrupole (by referring to "quad") and induced dipole (by referring to "idipole"). The contribution of induced dipole, permanent dipole and vdW are important to gA-ions and water-ions interactions owing to the close distance between permeation ions and gA or water. In the case of DMPC and bulk ions, the charge-related contribution is big. As similar as van der Waals interaction, the polarization-related, permanent dipole and quadrupole interactions are short-range interaction.

AMOEBA based polarizable force filed for DMPC molecule

```
##############################
##                          ##
##   Force Field Definition ##
##                          ##
##############################
```

forcefield	AMOEBA-DMPC
bond-cubic	-2.55
bond-quartic	3.793125
angle-cubic	-0.014
angle-quartic	0.000056
angle-pentic	-0.0000007
angle-sextic	0.000000022
torsionunit	0.5
vdwtype	BUFFERED-14-7
opbendtype	ALLINGER
opbend-cubic	-0.014
opbend-quartic	0.000056
opbend-pentic	-0.0000007
opbend-sextic	0.000000022
radiusrule	CUBIC-MEAN
radiustype	R-MIN
radiussize	DIAMETER
epsilonrule	HHG
dielectric	1.0
polarization	MUTUAL
vdw-12-scale	0.0
vdw-13-scale	0.0
vdw-14-scale	1.0
vdw-15-scale	1.0
mpole-12-scale	0.0
mpole-13-scale	0.0
mpole-14-scale	0.4
mpole-15-scale	0.8
polar-12-scale	0.0
polar-13-scale	0.0
polar-14-scale	1.0

```
polar-15-scale          1.0
polar-14-intra          0.5
direct-11-scale         0.0
direct-12-scale         1.0
direct-13-scale         1.0
direct-14-scale         1.0
mutual-11-scale         1.0
mutual-12-scale         1.0
mutual-13-scale         1.0
mutual-14-scale         1.0


      ##############################
      ##                          ##
      ##   Atom Type Definitions  ##
      ##                          ##
      ##############################


atom      1    1    N     "DMPC choline N+"       7    14.007    4
atom      2    2    C2    "DMPC choline C2"       6    12.011    4
atom      3    3    H2    "DMPC choline H2"       1     1.008    1
atom      4    2    C3    "DMPC choline C3"       6    12.011    4
atom      5    3    H3    "DMPC choline H3"       1     1.008    1
atom      6    2    C4    "DMPC choline C4"       6    12.011    4
atom      7    3    H4    "DMPC choline H4"       1     1.008    1
atom      8    4    C5    "DMPC choline C5"       6    12.011    4
atom      9    5    H5    "DMPC choline H5"       1     1.008    1
atom     10    6    C6    "DMPC choline C6"       6    12.011    4
atom     11    7    H6    "DMPC choline H6"       1     1.008    1
atom     12    8    O7    "DMPC phosphate O7"     8    15.999    2
atom     13    9    P8    "DMPC phosphate P8"    15    30.974    4
atom     14   10    O9    "DMPC phosphate O9"     8    15.999    1
atom     15   10    O10   "DMPC phosphate O10"    8    15.999    1
atom     16    8    O11   "DMPC phosphate O11"    8    15.999    2
atom     17    6    C12   "DMPC glycerol C12"     6    12.011    4
atom     18    7    H12   "DMPC glycerol H12"     1     1.008    1
atom     19   11    C13   "DMPC glycerol C13"     6    12.011    4
atom     20   12    H13   "DMPC glycerol H13"     1     1.008    1
atom     21   13    C14   "DMPC glycerol C14"     6    12.011    4
atom     22   14    H14   "DMPC glycerol H14"     1     1.008    1
atom     23   15    O15   "DMPC glycerol O15"     8    15.999    2
atom     24   22    O16   "DMPC glycerol O16"     8    15.999    2
atom     25   16    O1a   "DMPC sn-1 O1a"         8    15.999    1
```

atom	26	17	C1a	"DMPC acyl chaina C1"	6	12.011	3
atom	27	18	C2a	"DMPC acyl chaina C2"	6	12.011	4
atom	28	19	H2a	"DMPC acyl chaina H2"	1	1.008	1
atom	29	16	O1b	"DMPC sn-2 O1b"	8	15.999	1
atom	30	17	C1b	"DMPC acyl chainb C1"	6	12.011	3
atom	31	18	C2b	"DMPC acyl chainb C2"	6	12.011	4
atom	32	19	H2b	"DMPC acyl chainb H2"	1	1.008	1
atom	33	23	C3t	"DMPC acyl chainab C3"	6	12.011	4
atom	34	24	H3t	"DMPC acyl chainab H3"	1	1.008	1
atom	35	23	C4t	"DMPC acyl chainab C4"	6	12.011	4
atom	36	24	H4t	"DMPC acyl chainab H4"	1	1.008	1
atom	37	23	C5t	"DMPC acyl chainab C5"	6	12.011	4
atom	38	24	H5t	"DMPC acyl chainab H5"	1	1.008	1
atom	39	23	C6t	"DMPC acyl chainab C6"	6	12.011	4
atom	40	24	H6t	"DMPC acyl chainab H6"	1	1.008	1
atom	41	23	C7t	"DMPC acyl chainab C7"	6	12.011	4
atom	42	24	H7t	"DMPC acyl chainab H7"	1	1.008	1
atom	43	23	C8t	"DMPC acyl chainab C8"	6	12.011	4
atom	44	24	H8t	"DMPC acyl chainab H8"	1	1.008	1
atom	45	23	C9t	"DMPC acyl chainab C9"	6	12.011	4
atom	46	24	H9t	"DMPC acyl chainab H9"	1	1.008	1
atom	47	23	C10	"DMPC acyl chainab C10"	6	12.011	4
atom	48	24	H10	"DMPC acyl chainab H10"	1	1.008	1
atom	49	23	C11	"DMPC acyl chainab C11"	6	12.011	4
atom	50	24	H11	"DMPC acyl chainab H11"	1	1.008	1
atom	51	23	C12	"DMPC acyl chainab C12"	6	12.011	4
atom	52	24	H12	"DMPC acyl chainab H12"	1	1.008	1
atom	53	23	C13	"DMPC acyl chainab C13"	6	12.011	4
atom	54	24	H13	"DMPC acyl chainab H13"	1	1.008	1
atom	55	25	C14	"DMPC acyl chainab C14"	6	12.011	4
atom	56	26	H14	"DMPC acyl chainab H14"	1	1.008	1

```
################################
##                            ##
##   Van der Waals Parameters ##
##                            ##
################################
```

vdw	1	3.5245	0.0997

vdw	2	4.0110	0.1061	
vdw	3	3.1080	0.0252	0.920
vdw	4	3.6290	0.1061	
vdw	5	2.8120	0.0231	0.920
vdw	6	3.6290	0.1061	
vdw	7	2.8310	0.0228	0.920
vdw	8	3.5753	0.1045	
vdw	9	4.6725	0.3706	
vdw	10	3.4485	0.1176	
vdw	11	3.8325	0.0959	
vdw	12	3.1290	0.0228	0.940
vdw	13	4.0110	0.0959	
vdw	14	3.1290	0.0228	0.940
vdw	15	3.2347	0.1045	
vdw	16	3.4494	0.1176	
vdw	17	3.6290	0.1113	
vdw	18	3.6290	0.1061	
vdw	19	2.8310	0.0252	0.940
vdw	20	3.6500	0.1010	
vdw	21	2.5830	0.0260	0.920
vdw	22	3.2908	0.1155	
vdw	23	3.8200	0.1010	
vdw	24	2.9800	0.0240	0.920
vdw	25	3.8200	0.1010	
vdw	26	2.9600	0.0240	0.920

```
#################################
##                             ##
##   Bond Stretching Parameters   ##
##                             ##
#################################
```

bond	1	4	381.3	1.5224
bond	1	2	381.3	1.4977
bond	2	3	342.3	1.0736
bond	4	5	341.3	1.0738
bond	4	6	453.0	1.5478
bond	6	7	341.2	1.0809
bond	6	8	465.1	1.3730

bond	6	11	323.0	1.5226
bond	8	9	450.0	1.6292
bond	9	10	774.9	1.4693
bond	11	12	341.0	1.0782
bond	11	13	323.0	1.5145
bond	11	22	465.1	1.4266
bond	13	14	341.0	1.0811
bond	13	15	465.1	1.4109
bond	15	17	465.1	1.4216
bond	16	17	601.8	1.1796
bond	17	18	345.3	1.5124
bond	18	19	341.0	1.0868
bond	18	23	453.0	1.5280
bond	20	20	680.0	1.3201
bond	20	21	341.0	1.0810
bond	22	17	465.1	1.3194
bond	23	20	323.0	1.5053
bond	23	23	453.0	1.5312
bond	23	24	341.0	1.0868
bond	23	25	323.0	1.5299
bond	25	26	341.0	1.0861

```
#################################
##                             ##
##   Angle Bending Parameters  ##
##                             ##
#################################
```

angle	2	1	2	51.80	108.2200
angle	4	1	2	51.66	111.2200
angle	1	2	3	58.64	108.1800
angle	3	2	3	39.79	107.4500
angle	1	4	6	56.09	116.7300
angle	1	4	5	70.83	105.9500
angle	5	4	5	40.46	107.1900
angle	6	4	5	37.85	119.0991
angle	4	6	7	38.00	112.1434
angle	4	6	8	88.00	111.8635
angle	7	6	7	45.46	107.2300
angle	8	6	7	60.94	109.7200
angle	11	6	7	38.00	108.3774
angle	8	6	11	88.00	109.7000
angle	6	8	9	80.08	119.9600
angle	8	9	8	65.59	97.4600

angle	8	9	10	75.88	109.3400
angle	10	9	10	89.88	122.2200
angle	6	11	12	38.00	108.9840
angle	6	11	22	88.00	107.1000
angle	13	11	6	60.00	114.2619
angle	13	11	12	38.00	107.6051
angle	13	11	22	88.00	106.3800
angle	22	11	12	60.99	108.4800
angle	11	13	14	38.00	110.9000
angle	11	13	15	88.00	109.7000
angle	14	13	14	39.57	108.5300
angle	14	13	15	60.99	109.7500
angle	13	15	17	88.50	117.3500
angle	16	17	15	50.00	123.2900
angle	18	17	16	60.00	125.2800
angle	18	17	15	60.00	111.3000
angle	16	17	22	50.00	123.7800
angle	22	17	18	60.00	111.0300
angle	17	18	19	38.00	107.4700
angle	17	18	23	48.20	112.9900
angle	19	18	19	45.57	105.8700
angle	19	18	23	38.00	111.4841
angle	20	20	21	32.00	118.8892
angle	23	20	20	60.00	125.4116
angle	23	20	21	32.00	115.6966
angle	11	22	17	88.50	118.9300
angle	18	23	24	38.00	107.9848
angle	18	23	23	48.20	112.2989
angle	23	23	20	48.20	112.8390
angle	24	23	20	38.00	108.7346
angle	23	23	23	48.25	113.3100
angle	23	23	24	37.99	109.4700
angle	24	23	24	39.66	106.2700
angle	24	23	25	37.99	109.3700
angle	23	23	25	48.29	112.8700
angle	23	25	26	42.42	111.2700
angle	26	25	26	39.51	107.6500

```
################################
##                            ##
##   Stretch-Bend Parameters  ##
##                            ##
################################
```

strbnd	2	1	2	7.20	7.20
strbnd	4	1	2	7.20	7.20
strbnd	1	2	3	11.50	11.50
strbnd	1	4	6	18.70	18.70
strbnd	1	4	5	11.50	11.50
strbnd	6	4	5	11.50	18.70
strbnd	4	6	8	18.70	18.70
strbnd	4	6	7	11.50	18.70
strbnd	8	6	7	-4.50	38.00
strbnd	11	6	7	11.50	11.50
strbnd	8	6	11	18.70	18.70
strbnd	8	6	12	-4.50	38.00
strbnd	8	6	15	18.70	18.70
strbnd	8	6	17	18.70	18.70
strbnd	11	6	12	11.50	11.50
strbnd	15	6	12	-4.50	38.00
strbnd	15	6	7	-4.50	38.00
strbnd	17	6	7	11.50	18.70
strbnd	17	6	11	18.70	18.70
strbnd	17	6	12	11.50	18.70
strbnd	17	6	15	18.70	18.70
strbnd	8	7	6	38.00	38.00
strbnd	6	8	7	-4.50	38.00
strbnd	6	8	9	38.00	38.00
strbnd	6	8	13	38.00	38.00
strbnd	9	8	7	-4.50	38.00
strbnd	9	8	13	38.00	38.00
strbnd	22	8	9	38.00	38.00
strbnd	22	8	5	38.00	38.00
strbnd	22	8	7	-4.50	38.00
strbnd	8	9	8	8.60	8.60
strbnd	8	9	10	8.60	8.60
strbnd	8	9	23	8.60	8.60
strbnd	8	9	24	8.60	8.60
strbnd	23	9	10	8.60	8.60
strbnd	23	9	24	8.60	8.60
strbnd	24	9	10	8.60	8.60
strbnd	6	11	12	11.50	18.70
strbnd	6	11	13	18.70	18.70
strbnd	6	11	18	18.70	18.70
strbnd	6	11	22	18.70	18.70
strbnd	13	11	12	11.50	18.70
strbnd	13	11	18	18.70	18.70
strbnd	13	11	22	18.70	18.70

strbnd	15	11	18	18.70	18.70
strbnd	15	11	22	18.70	18.70
strbnd	15	11	12	-4.50	38.00
strbnd	18	11	12	11.50	18.70
strbnd	22	11	12	-4.50	38.00
strbnd	22	11	18	18.70	18.70
strbnd	6	12	11	38.00	38.00
strbnd	8	13	10	18.70	18.70
strbnd	8	13	22	18.70	18.70
strbnd	8	13	11	18.70	18.70
strbnd	10	13	15	18.70	18.70
strbnd	11	13	10	18.70	18.70
strbnd	11	13	14	11.50	18.70
strbnd	11	13	15	18.70	18.70
strbnd	14	13	8	-4.50	38.00
strbnd	14	13	10	-4.50	38.00
strbnd	14	13	15	-4.50	38.00
strbnd	14	13	22	-4.50	38.00
strbnd	15	14	13	38.00	38.00
strbnd	15	13	22	18.70	18.70
strbnd	22	13	11	18.70	18.70
strbnd	22	13	10	18.70	18.70
strbnd	6	15	11	38.00	38.00
strbnd	6	15	13	38.00	38.00
strbnd	6	15	17	38.00	38.00
strbnd	6	15	14	-4.50	38.00
strbnd	11	15	17	38.00	38.00
strbnd	11	15	14	-4.50	38.00
strbnd	13	15	11	38.00	38.00
strbnd	13	15	14	-4.50	38.00
strbnd	13	15	17	38.00	38.00
strbnd	14	15	17	-4.50	38.00
strbnd	17	16	18	38.00	38.00
strbnd	17	16	19	-4.50	38.00
strbnd	18	16	19	-4.50	38.00
strbnd	6	17	15	18.70	18.70
strbnd	16	17	15	18.70	18.70
strbnd	16	17	24	-4.50	38.00
strbnd	18	17	16	18.70	18.70
strbnd	18	17	22	18.70	18.70
strbnd	18	17	24	11.50	11.50
strbnd	18	17	15	18.70	18.70
strbnd	18	17	6	18.70	18.70
strbnd	18	17	18	18.70	18.70

strbnd	22	17	24	-4.50	38.00
strbnd	11	18	19	11.50	18.70
strbnd	11	18	23	18.70	18.70
strbnd	16	18	17	18.70	18.70
strbnd	16	18	11	18.70	18.70
strbnd	16	18	19	-4.50	38.00
strbnd	16	18	23	18.70	18.70
strbnd	17	18	11	18.70	18.70
strbnd	17	18	19	11.50	18.70
strbnd	17	18	23	18.70	18.70
strbnd	17	18	17	18.70	18.70
strbnd	23	18	19	11.50	18.70
strbnd	19	18	23	11.50	18.70
strbnd	16	19	18	38.00	38.00
strbnd	23	19	18	38.00	38.00
strbnd	21	20	20	11.50	18.70
strbnd	23	20	21	11.50	18.70
strbnd	8	22	17	38.00	38.00
strbnd	8	22	13	38.00	38.00
strbnd	8	22	11	38.00	38.00
strbnd	17	22	13	38.00	38.00
strbnd	17	22	11	38.00	38.00
strbnd	13	22	11	38.00	38.00
strbnd	9	23	18	18.70	18.70
strbnd	9	23	19	11.50	18.70
strbnd	9	24	23	38.00	38.00
strbnd	9	23	24	11.50	18.70
strbnd	18	23	19	11.50	18.70
strbnd	18	23	24	11.50	18.70
strbnd	18	23	23	18.70	18.70
strbnd	20	23	20	18.70	18.70
strbnd	20	23	21	11.50	11.50
strbnd	23	23	20	18.70	18.70
strbnd	23	23	24	11.50	18.70
strbnd	23	23	23	18.70	18.70
strbnd	23	25	26	11.50	11.50
strbnd	24	23	20	11.50	18.70
strbnd	25	23	24	11.50	18.70
strbnd	17	24	23	38.00	38.00

```
#####################################
##                                 ##
##   Out-of-Plane Bend Parameters  ##
```

```
##                                    ##
#####################################
```

opbend	18	17	0	0	14.402
opbend	15	17	0	0	14.402
opbend	22	17	0	0	14.402
opbend	16	17	0	0	47.761

```
############################
 ##                        ##
 ##   Torsional Parameters ##
 ##                        ##
 ############################
```

torsion	3	2	1	4	0.072	0.0	1	-0.012	180.0	2	0.563	0.0 3
torsion	3	2	1	2	0.072	0.0	1	-0.012	180.0	2	0.563	0.0 3
torsion	1	4	6	7	0.000	0.0	1	0.000	180.0	2	0.341	0.0 3
torsion	1	4	6	8	6.837	0.0	1	0.630	180.0	2	4.030	0.0 3
torsion	5	4	1	2	0.000	0.0	1	0.000	180.0	2	0.341	0.0 3
torsion	5	4	6	7	0.000	0.0	1	0.000	180.0	2	0.299	0.0 3
torsion	5	4	6	8	0.000	0.0	1	0.000	180.0	2	0.341	0.0 3
torsion	6	4	1	2	0.000	0.0	1	-1.747	180.0	2	-0.160	0.0 3
torsion	4	6	8	9	-12.340	0.0	1	0.372	180.0	2	0.499	0.0 3
torsion	7	6	8	9	0.000	0.0	1	0.000	180.0	2	0.120	0.0 3
torsion	7	6	11	12	0.000	0.0	1	0.000	180.0	2	0.299	0.0 3
torsion	7	6	11	13	0.000	0.0	1	0.000	180.0	2	0.341	0.0 3
torsion	7	6	11	22	0.000	0.0	1	0.000	180.0	2	0.341	0.0 3
torsion	8	6	11	12	0.000	0.0	1	0.000	180.0	2	0.341	0.0 3
torsion	8	6	11	13	2.463	0.0	1	1.728	180.0	2	4.623	0.0 3
torsion	8	6	11	22	-2.710	0.0	1	-3.783	180.0	2	4.470	0.0 3
torsion	9	8	6	11	2.772	0.0	1	-2.683	180.0	2	-0.886	0.0 3
torsion	8	9	8	6	0.885	0.0	1	-2.896	180.0	2	0.281	0.0 3
torsion	10	9	8	6	-6.338	0.0	1	6.788	180.0	2	0.370	0.0 3
torsion	6	11	22	17	6.291	0.0	1	-0.504	180.0	2	-7.493	0.0 3
torsion	12	11	22	17	0.000	0.0	1	0.000	180.0	2	0.341	0.0 3
torsion	13	11	22	17	-1.524	0.0	1	0.086	180.0	2	1.320	0.0 3
torsion	11	13	15	17	-2.616	0.0	1	-0.983	180.0	2	-0.373	0.0 3
torsion	14	13	11	6	0.000	0.0	1	0.000	180.0	2	0.341	0.0 3
torsion	14	13	11	12	0.000	0.0	1	0.000	180.0	2	0.299	0.0 3
torsion	14	13	11	15	0.000	0.0	1	0.000	180.0	2	0.341	0.0 3

torsion	14	13	15	17	0.000 0.0 1	0.000 180.0 2	0.341 0.0 3
torsion	14	13	11	22	0.000 0.0 1	0.000 180.0 2	0.341 0.0 3
torsion	15	13	11	6	0.814 0.0 1	0.430 180.0 2	1.142 0.0 3
torsion	15	13	11	12	0.000 0.0 1	0.000 180.0 2	0.341 0.0 3
torsion	15	13	11	22	1.540 0.0 1	-0.733 180.0 2	0.965 0.0 3
torsion	19	18	17	15	0.000 0.0 1	0.000 180.0 2	0.341 0.0 3
torsion	19	18	17	16	-0.154 0.0 1	0.044 180.0 2	-0.086 0.0 3
torsion	19	18	17	22	0.000 0.0 1	0.000 180.0 2	0.341 0.0 3
torsion	18	17	15	13	0.000 0.0 1	12.167 180.0 2	-4.198 0.0 3
torsion	16	17	15	13	0.000 0.0 1	0.000 180.0 2	-5.888 0.0 3
torsion	18	17	22	11	0.000 0.0 1	6.721 180.0 2	0.000 0.0 3
torsion	15	17	18	23	1.231 0.0 1	0.000 180.0 2	0.000 0.0 3
torsion	16	17	18	23	0.000 0.0 1	-0.039 180.0 2	0.000 0.0 3
torsion	22	17	18	23	0.000 0.0 1	-0.039 180.0 2	0.000 0.0 3
torsion	17	18	23	23	1.532 0.0 1	-1.981 180.0 2	1.641 0.0 3
torsion	17	18	23	24	0.000 0.0 1	0.000 180.0 2	0.341 0.0 3
torsion	19	18	23	23	0.000 0.0 1	0.000 180.0 2	0.341 0.0 3
torsion	19	18	23	24	0.000 0.0 1	0.000 180.0 2	0.299 0.0 3
torsion	21	20	20	21	0.000 0.0 1	4.070 180.0 2	0.000 0.0 3
torsion	23	20	20	21	0.000 0.0 1	6.100 180.0 2	0.000 0.0 3
torsion	23	20	20	23	0.000 0.0 1	8.000 180.0 2	0.000 0.0 3
torsion	11	22	17	16	0.000 0.0 1	6.721 180.0 2	0.000 0.0 3
torsion	23	23	20	20	2.775 0.0 1	-0.695 180.0 2	-1.271 0.0 3
torsion	23	23	20	21	0.000 0.0 1	0.000 180.0 2	0.341 0.0 3
torsion	24	23	20	20	0.000 0.0 1	0.000 180.0 2	0.341 0.0 3
torsion	24	23	20	21	0.000 0.0 1	0.000 180.0 2	0.299 0.0 3
torsion	18	23	23	23	2.818 0.0 1	-0.410 180.0 2	2.472 0.0 3
torsion	18	23	23	24	0.000 0.0 1	0.000 180.0 2	0.341 0.0 3
torsion	23	23	23	20	0.649 0.0 1	0.419 180.0 2	2.472 0.0 3
torsion	23	23	23	23	0.568 0.0 1	-0.375 180.0 2	2.302 0.0 3
torsion	23	23	23	24	0.000 0.0 1	0.000 180.0 2	0.341 0.0 3
torsion	23	23	23	25	0.717 0.0 1	-0.133 180.0 2	1.123 0.0 3
torsion	24	23	23	20	0.000 0.0 1	0.000 180.0 2	0.341 0.0 3
torsion	24	23	23	24	0.000 0.0 1	0.000 180.0 2	0.299 0.0 3
torsion	24	23	23	25	0.000 0.0 1	0.000 180.0 2	0.341 0.0 3
torsion	26	25	23	23	0.000 0.0 1	0.000 180.0 2	0.341 0.0 3
torsion	26	25	23	24	0.000 0.0 1	0.000 180.0 2	0.299 0.0 3

```
#####################################
##                                 ##
##   Atomic Multipole Parameters   ##
##                                 ##
#####################################
```

multipole	1	2	0	0.33714		
				0.00245	-0.00012	-0.00175
				0.08092		
				-0.01215	-0.15867	
				-0.00549	0.00028	0.07775
multipole	2	1	3	-0.11686		
				0.00000	0.00000	0.31787
				-0.60382		
				0.00000	-0.58497	
				0.00000	0.00000	1.18879
multipole	3	2	1	0.09694		
				-0.02570	0.00000	-0.11448
				-0.01851		
				0.00000	0.05789	
				-0.01324	0.00000	-0.03938
multipole	4	1	5	-0.11686		
				0.00000	0.00000	0.31787
				-0.60382		
				0.00000	-0.58497	
				0.00000	0.00000	1.18879
multipole	5	4	1	0.09694		
				-0.02570	0.00000	-0.11448
				-0.01851		
				0.00000	0.05789	
				-0.01324	0.00000	-0.03938
multipole	6	1	7	-0.11686		
				0.00000	0.00000	0.31787
				-0.60382		
				0.00000	-0.58497	
				0.00000	0.00000	1.18879
multipole	7	6	1	0.09694		
				-0.02570	0.00000	-0.11448
				-0.01851		
				0.00000	0.05789	
				-0.01324	0.00000	-0.03938
multipole	8	1	10	-0.11694		
				0.22113	0.00000	0.59083
				-0.40092		
				0.00000	-0.58589	
				-0.07374	0.00000	0.98681
multipole	9	8	1	0.09783		
				-0.02013	0.00000	-0.03076
				-0.05865		

				0.00000	0.12686	
				0.00231	0.00000	-0.06821
multipole	10	8	12	0.12911		
				0.38278	0.00000	0.02972
				0.46586		
				0.00000	-0.33559	
				-0.77999	0.00000	-0.13027
multipole	11	10	8	0.02153		
				-0.03930	0.00000	-0.08206
				0.11430		
				0.00000	-0.05779	
				-0.05876	0.00000	-0.05651
multipole	12	10	13	-0.53623		
				0.05021	0.00000	0.36055
				-0.59680		
				0.00000	-0.94938	
				-0.46030	0.00000	1.54618
multipole	13	12	-16	1.75680		
				0.00000	0.00000	0.04602
				0.23769		
				0.00000	0.43507	
				0.00000	0.00000	-0.67276
multipole	14	13	12	-0.94505		
				0.00000	0.00000	-0.15325
				-0.04763		
				0.00000	-0.22894	
				0.00000	0.00000	0.27657
multipole	15	13	16	-0.94505		
				0.00000	0.00000	-0.09516
				0.08015		
				0.00000	-0.40113	
				0.00000	0.00000	0.32098
multipole	16	17	13	-0.53623		
				-0.00092	0.00000	0.29349
				0.29881		
				0.00000	-0.83620	
				-0.52150	0.00000	0.53739
multipole	17	19	21	0.12911		
				0.23887	0.00000	0.07616
				-0.10304		
				0.00000	-0.10267	
				0.92424	0.00000	0.20571
multipole	18	17	19	0.02153		
				0.02261	0.00000	0.08329

				-0.03877		
				0.00000	-0.21786	
				-0.01836	0.00000	0.25663
multipole	19	21	17	0.02850		
				0.07077	0.00000	0.19142
				-0.18886		
				0.00000	-0.05163	
				-0.37242	0.00000	0.24049
multipole	20	19	21	0.08536		
				-0.03266	0.00000	0.05235
				-0.02202		
				0.00000	-0.03428	
				-0.03396	0.00000	0.05630
multipole	21	19	23	0.08549		
				0.34394	0.00000	0.17112
				0.35890		
				0.00000	-0.54665	
				-0.69386	0.00000	0.18775
multipole	22	21	19	0.03662		
				-0.03861	0.00000	-0.06411
				-0.05043		
				0.00000	0.05366	
				0.04566	0.00000	-0.00323
multipole	23	21	26	-0.36349		
				0.10244	0.00000	0.33467
				-0.41600		
				0.00000	-0.80950	
				-0.46144	0.00000	1.22550
multipole	24	19	30	-0.29002		
				0.02377	0.00000	0.33600
				-0.46319		
				0.00000	-0.27652	
				-0.38655	0.00000	0.73971
multipole	25	26	27	-0.67210		
				-0.09291	0.00000	-0.07763
				-0.47139		
				0.00000	0.21519	
				0.00058	0.00000	0.25620
multipole	26	27	23	0.96736		
				-0.12879	0.00000	-0.00436
				0.52049		
				0.00000	-0.16842	
				-0.36073	0.00000	-0.35207
multipole	27	33	26	-0.33625		

				-0.09089	0.00000	0.29751
				-0.27800		
				0.00000	-0.39864	
				0.01209	0.00000	0.67664
multipole	28	27	33	0.08282		
				0.06762	0.00000	-0.12677
				0.08315		
				0.00000	0.07614	
				0.09300	0.00000	-0.15929
multipole	29	30	31	-0.62676		
				0.01952	0.00000	-0.06997
				-0.35428		
				0.00000	0.11982	
				0.15384	0.00000	0.23446
multipole	30	31	24	0.78858		
				-0.02215	0.00000	-0.30454
				0.01893		
				0.00000	-0.05943	
				-0.50046	0.00000	0.04050
multipole	31	33	30	-0.15457		
				0.18371	0.00000	0.20868
				0.21424		
				0.00000	-0.55972	
				-0.14259	0.00000	0.34548
multipole	32	31	33	0.08635		
				0.03754	0.00000	-0.11117
				0.01891		
				0.00000	0.06980	
				-0.00128	0.00000	-0.08871
multipole	33	35	27	-0.12028		
				0.00000	0.00000	0.08920
				-0.45259		
				0.00000	0.22212	
				0.00000	0.00000	0.23047
multipole	33	35	31	-0.12028		
				0.00000	0.00000	0.08920
				-0.45259		
				0.00000	0.22212	
				0.00000	0.00000	0.23047
multipole	34	33	35	0.06014		
				-0.02503	0.00000	0.07942
				-0.13076		
				0.00000	-0.05780	
				-0.05505	0.00000	0.18856

```
multipole    35    37    33              -0.12028
                                           0.00000    0.00000    0.33839
                                          -0.68115
                                           0.00000    0.10340
                                           0.00000    0.00000    0.57775
multipole    36    35    37               0.06014
                                           0.00661    0.00000    0.11930
                                          -0.16797
                                           0.00000   -0.07505
                                           0.12169    0.00000    0.24302
multipole    37    35    39              -0.12028
                                           0.00000    0.00000    0.14448
                                          -0.28128
                                           0.00000   -0.00441
                                           0.00000    0.00000    0.28569
multipole    38    37    35               0.06014
                                           0.01615    0.00000    0.22955
                                          -0.21643
                                           0.00000   -0.20428
                                           0.02788    0.00000    0.42071
multipole    39    37    41              -0.12028
                                           0.00000    0.00000   -0.01354
                                          -0.04975
                                           0.00000    0.10300
                                           0.00000    0.00000   -0.05325
multipole    40    39    37               0.06014
                                           0.04578    0.00000    0.17404
                                          -0.16537
                                           0.00000   -0.18492
                                           0.07403    0.00000    0.35029
multipole    41    39    43              -0.12028
                                           0.00000    0.00000   -0.05085
                                          -0.30712
                                           0.00000    0.15148
                                           0.00000    0.00000    0.15564
multipole    42    41    39               0.06014
                                           0.08671    0.00000    0.09820
                                          -0.08927
                                           0.00000   -0.11428
                                           0.11609    0.00000    0.20355
multipole    43    41   -45              -0.12028
                                           0.00000    0.00000   -0.02523
                                           0.11672
                                           0.00000    0.26467
```

0.00000 0.00000 -0.38139
multipole 44 43 41 0.06014
-0.00822 0.00000 0.09256
-0.12801
0.00000 -0.10497
-0.03016 0.00000 0.23298
multipole 45 47 43 -0.12028
0.00000 0.00000 0.04373
-0.11409
0.00000 0.25407
0.00000 0.00000 -0.13998
multipole 46 45 47 0.06014
0.03147 0.00000 0.10815
-0.04700
0.00000 -0.16314
0.06910 0.00000 0.21014
multipole 47 49 45 -0.12028
0.00000 0.00000 0.04534
0.03346
0.00000 0.20973
0.00000 0.00000 -0.24319
multipole 48 47 49 0.06014
0.02363 0.00000 0.17973
-0.11928
0.00000 -0.23560
0.06988 0.00000 0.35488
multipole 49 51 47 -0.12028
0.00000 0.00000 0.19090
-0.13792
0.00000 0.13912
0.00000 0.00000 -0.00120
multipole 50 49 51 0.06014
-0.00563 0.00000 0.24246
-0.19465
0.00000 -0.25447
0.03243 0.00000 0.44912
multipole 51 49 53 -0.12028
0.00000 0.00000 0.17802
-0.14130
0.00000 -0.03152
0.00000 0.00000 0.17282
multipole 52 51 49 0.06014
0.01343 0.00000 0.22793
-0.19168

```
                                        0.00000     -0.23346
                                        0.05530      0.00000      0.42514
multipole     53    51    55          -0.12028
                                        0.00000      0.00000     -0.04785
                                       -0.24581
                                        0.00000     -0.05659
                                        0.00000      0.00000      0.30240
multipole     54    53    51           0.06014
                                        0.10189      0.00000      0.12283
                                       -0.11650
                                        0.00000     -0.13166
                                        0.14624      0.00000      0.24816
multipole     55    53    56          -0.16638
                                        0.00000      0.00000      0.13817
                                        0.23776
                                        0.00000      0.30333
                                        0.00000      0.00000     -0.54109
multipole     56    55    53           0.05546
                                       -0.02203      0.00000      0.07426
                                       -0.02038
                                        0.00000     -0.17435
                                       -0.01461      0.00000      0.19473


        ########################################
        ##                                    ##
        ##   Dipole Polarizability Parameters ##
        ##                                    ##
        ########################################


polarize    1    1.073      0.390    2    4    6    8
polarize    2    1.334      0.390    1    3
polarize    3    0.496      0.390    2
polarize    4    1.334      0.390    1    5
polarize    5    0.496      0.390    4
polarize    6    1.334      0.390    1    7
polarize    7    0.496      0.390    6
polarize    8    1.334      0.390    1    9
polarize    9    0.496      0.390    8
polarize    10    1.334      0.390    11    12
polarize    11    0.496      0.390    10
polarize    12    0.837      0.390    10    13
polarize    13    1.828      0.390    12    14    15    16
polarize    14    0.837      0.390    13
```

polarize	15	0.837	0.390	13		
polarize	16	0.837	0.390	13	17	
polarize	17	1.334	0.390	16	18	
polarize	18	0.496	0.390	17		
polarize	19	1.334	0.390	20	24	
polarize	20	0.496	0.390	19		
polarize	21	1.334	0.390	22	23	
polarize	22	0.496	0.390	21		
polarize	23	0.837	0.390	21	26	
polarize	24	0.837	0.390	30	19	
polarize	25	0.837	0.390	26		
polarize	26	1.334	0.390	23	27	25
polarize	27	1.334	0.390	26	28	
polarize	28	0.496	0.390	27		
polarize	29	0.837	0.390	30		
polarize	30	1.334	0.390	29	24	31
polarize	31	1.334	0.390	30	32	
polarize	32	0.496	0.390	31		
polarize	33	1.334	0.390	34		
polarize	34	0.496	0.390	33		
polarize	35	1.334	0.390	36		
polarize	36	0.496	0.390	35		
polarize	37	1.334	0.390	38		
polarize	38	0.496	0.390	37		
polarize	39	1.334	0.390	40		
polarize	40	0.496	0.390	39		
polarize	41	1.334	0.390	42		
polarize	42	0.496	0.390	41		
polarize	43	1.334	0.390	44		
polarize	44	0.496	0.390	43		
polarize	45	1.334	0.390	46		
polarize	46	0.496	0.390	45		
polarize	47	1.334	0.390	48		
polarize	48	0.496	0.390	47		
polarize	49	1.334	0.390	50		
polarize	50	0.496	0.390	49		
polarize	51	1.334	0.390	52		
polarize	52	0.496	0.390	51		
polarize	53	1.334	0.390	54		
polarize	54	0.496	0.390	53		
polarize	55	1.334	0.390	56		
polarize	56	0.496	0.390	55		