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

Supporting Information for Simulating the binding of organic functional groups to aqueous calcium carbonate species

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S1. SUPPLEMENTARY FIGURE

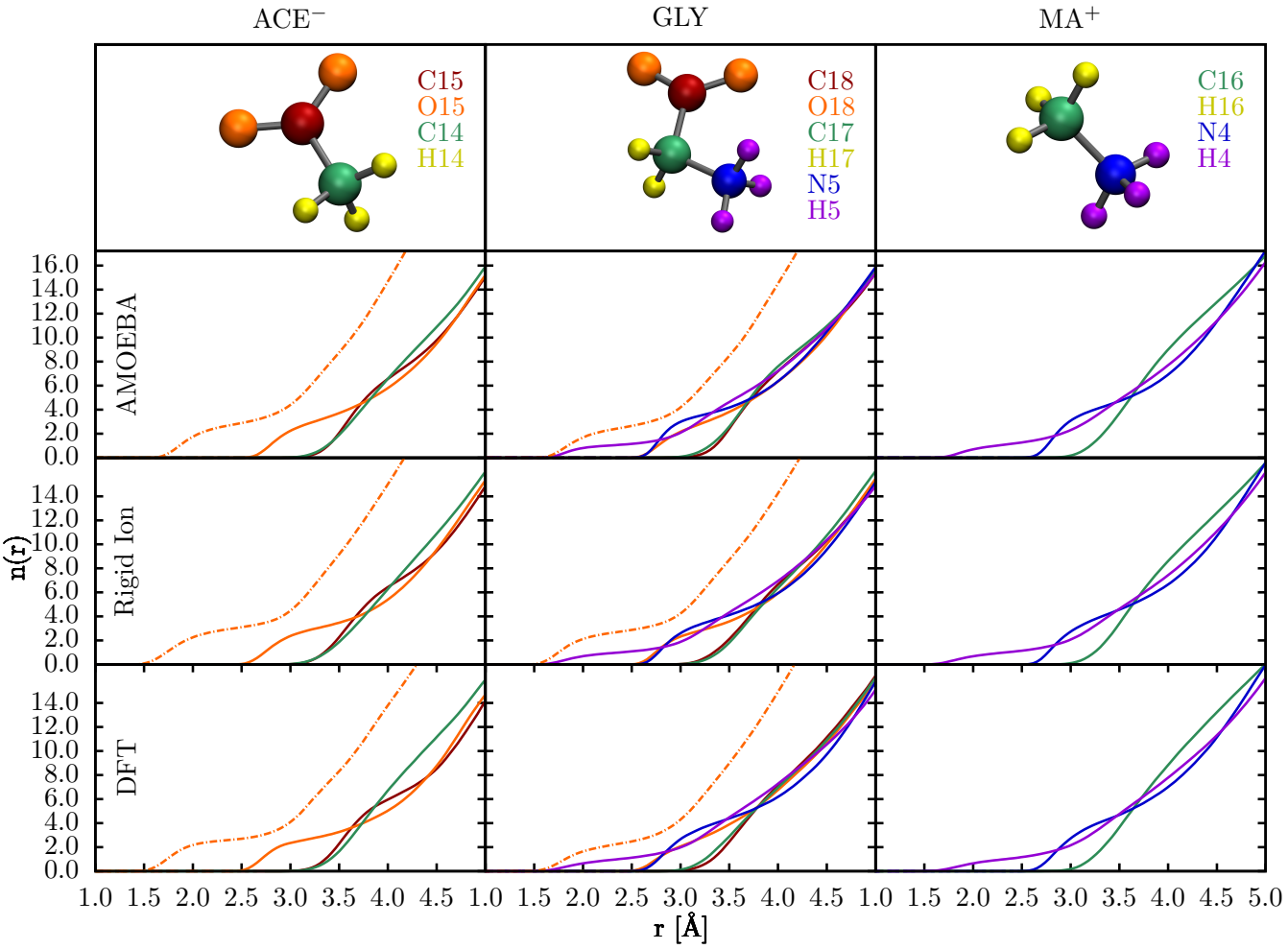

FIG. S1. Integrals of the radial distribution functions (coordination numbers, n(r)) for acetate (ACE-), the glycine zwitterion (GLY) and methylammonium (MA+) in water obtained from molecular dynamics simulation. The solid and dashed lines are for O_w and H_w, respectively, with curves colour-coded to reflect the atom of the molecule whose radial distribution function is being shown, as per the scheme given. For clarity, curves are only shown for those atoms where there are significant peaks observed.

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S2. FORCE FIELD PARAMETERS FOR POLARISABLE AMOEBA MODEL

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           q11=" 0.000343315"
           q21=" 0.000000000" q22="-0.000059833"
           q31=" 0.000096171" q32=" 0.000000000" q33="-0.000283482"  />
<Multipole type="34" kz="33" kx="34"
           c0 ="-0.946070000"
           d1 =" 0.005137782" d2 =" 0.000000000" d3 ="-0.000298456"
           q11="-0.000419212"
           q21=" 0.000000000" q22="-0.000063464"
           q31=" 0.000036040" q32=" 0.000000000" q33=" 0.000482676"  />

<Polarize type="1"  polarizability="0.000837" thole="0.39" pgrp1="2" />
<Polarize type="2"  polarizability="0.000496" thole="0.39" pgrp1="1" />
<Polarize type="3"  polarizability="0.000550" thole="0.16" />
<Polarize type="11" polarizability="0.001334" thole="0.39" pgrp1="12" />
<Polarize type="12" polarizability="0.000837" thole="0.39" pgrp1="11" />
<Polarize type="21" polarizability="0.001334" thole="0.39" />
<Polarize type="22" polarizability="0.000496" thole="0.39" />
<Polarize type="23" polarizability="0.001334" thole="0.39" />
<Polarize type="24" polarizability="0.000921" thole="0.39" />
<Polarize type="25" polarizability="0.001073" thole="0.39" />
<Polarize type="26" polarizability="0.000496" thole="0.39" />
```

```
  <Polarize type="27" polarizability="0.001334" thole="0.39" />
  <Polarize type="28" polarizability="0.000496" thole="0.39" />
  <Polarize type="29" polarizability="0.001073" thole="0.39" />
  <Polarize type="30" polarizability="0.000496" thole="0.39" />
  <Polarize type="31" polarizability="0.001334" thole="0.39" />
  <Polarize type="32" polarizability="0.000496" thole="0.39" />
  <Polarize type="33" polarizability="0.001334" thole="0.39" />
  <Polarize type="34" polarizability="0.000837" thole="0.39" />
  </AmoebaMultipoleForce>

<!-- Urey-Bradley term for water, units kj/mol/nm^2 | conversion factor: 418.4 -->
-->
 <AmoebaUreyBradleyForce cubic="0.0" quartic="0.0"  >
  <UreyBradley class1="2" class2="1" class3="2" k="-3179.84" d="0.15326" />
 </AmoebaUreyBradleyForce>

</ForceField>
```

S3. FORCE FIELD PARAMETERS FOR RIGID-ION MODEL

```
##############################################################################################
# Library file for minerals simulations with LAMMPS
# It includes potentials for
# water (SPC/FW)
# Alkaline and alkaline-earth metals
# carbonate
# acetate, methylammonium, glycine
##############################################################################################
##############################################################################################
#### Atoms' types - mass - charge
##############################################################################################
#@ 48   atom types

# Monovalent ions
variable Na  equal  1  # sodium
variable K   equal  2  # potassium
variable Rb  equal  3  # rubidium
variable Cs  equal  4  # cesium
variable Cl  equal  5  # chloride

# Divalent ions
variable Mg  equal  6  # magnesium
variable Ca  equal  7  # calcium
variable Sr  equal  8  # strontium
variable Ba  equal  9  # barium

# Water - SPC/Fw
variable O2  equal 12  # water
variable H2  equal 13  #

# Carbonate
variable C4  equal 16  # carbonate
variable O4  equal 17  #

# Acetate
variable C14 equal 35  #
variable H14 equal 36  #
variable C15 equal 37  #
variable O15 equal 38  #

# Methylammonium
variable C16 equal 39  #
variable H4  equal 40  #
variable H16 equal 41  #
variable N4  equal 42  #

# Glycine (ZT)
variable C17 equal 43  #
variable C18 equal 44  #
variable H5  equal 45  #
variable H17 equal 46  #
variable N5  equal 47  #
variable O18 equal 48  #

##############################################################################################
#### Atomic masses
##############################################################################################

mass ${Na}  22.990
mass ${K}   39.100
mass ${Rb}  85.470
mass ${Cs} 132.900
mass ${Cl}  35.450
mass ${Mg}  24.310
mass ${Ca}  40.080
mass ${Sr}  87.620
mass ${Ba} 137.330
mass ${O2}  16.000
mass ${H2}   1.010
mass ${C4}  12.010
mass ${O4}  16.000

# Acetate
mass ${C14} 12.010
mass ${H14} 1.0100
mass ${C15} 12.010
mass ${O15} 16.000

# Methylammonium
mass ${H4}   1.008
mass ${N4}  14.010
mass ${C16} 12.010
mass ${H16}  1.008

# Glycine (ZT)
```

```
mass ${H5}   1.008
mass ${O18} 16.000
mass ${C18} 12.011
mass ${H17}  1.008
mass ${C17} 12.011
mass ${N5}  14.0067

##############################################################################################
#### Atomic charges
##############################################################################################

set type ${Na}  charge     1.000000
set type ${K}   charge     1.000000
set type ${Rb}  charge     1.000000
set type ${Cs}  charge     1.000000
set type ${Cl}  charge    -1.000000
set type ${Mg}  charge     2.000000
set type ${Ca}  charge     2.000000
set type ${Sr}  charge     2.000000
set type ${Ba}  charge     2.000000

# Water SPC/Fw
set type ${O2}  charge    -0.820000
set type ${H2}  charge     0.410000

# Carbonate
set type ${C4}  charge     1.123285
set type ${O4}  charge    -1.041095

# Acetate
set type ${C14} charge    -0.348000
set type ${H14} charge     0.064000
set type ${C15} charge     0.764000
set type ${O15} charge    -0.804000

# Methylammonium
set type ${C16} charge    -0.079000
set type ${H4}  charge     0.311000
set type ${H16} charge     0.111000
set type ${N4}  charge    -0.187000

# Glycine (ZT)
set type ${H5}  charge     0.307000
set type ${O18} charge    -0.733000
set type ${C18} charge     0.611000
set type ${H17} charge     0.082000
set type ${C17} charge    -0.043000
set type ${N5}  charge    -0.187000

##############################################################################################
#### Covalent bond parameters
##############################################################################################
#@  13   bond types

bond_style  hybrid harmonic morse
#@ O2 - H2
bond_coeff   1   harmonic    22.965000      1.0120000
#@ C4 - O4
bond_coeff   2   harmonic    20.424650      1.3042000

# Acetate
#@ H14  - C14
bond_coeff   3   harmonic    15.618400      1.0963000
#@ C15  - O15
bond_coeff   4   harmonic    24.765100      1.2516000
#@ C14  - C15
bond_coeff   5   harmonic    11.482000      1.5768500

# Methylammonium
#@ C16  - H16
bond_coeff   6   harmonic    16.905200      1.0876000
#@ N4  - C16
bond_coeff   7   harmonic    13.162300      1.4958000
#@ N4  - H4
bond_coeff   8   harmonic    20.528750      1.0250000

# Glycine (ZT)
#@ C17  - H17
bond_coeff   9   harmonic    15.618400      1.0963000
#@ O18  - C18
bond_coeff  10   harmonic    24.765100      1.2516000
#@ C17  - N5
bond_coeff  11   harmonic    13.162300      1.4658000
#@ N5  - H5
bond_coeff  12   harmonic    20.528750      1.0250000
#@ C18  - C17
bond_coeff  13   harmonic    11.482000      1.5100000

##############################################################################################
#### Covalent angle-bending parameters
##############################################################################################
#@ 18 angle types

angle_style  hybrid class2   harmonic
#@ H2 - O2 - H2
angle_coeff   1   harmonic    1.6456800    113.24000
#@ O4 - C4 - O4
angle_coeff   2   class2      120.00000      6.6170000      0.0000000      0.0000000
angle_coeff   2   class2 bb    12.81800      1.3042000      1.3042000
angle_coeff   2   class2 ba     1.53319      1.5331900      1.3042000      1.3042000

# Acetate
#@ H14  - C14  - H14
angle_coeff   3   harmonic     1.5441000      108.57000
#@ C14  - C15  - O15
angle_coeff   4   harmonic     2.8160500      115.04000
#@ O15  - C15  - O15
angle_coeff   5   harmonic     5.0780000      129.92000
#@ H14  - C14  - C15
angle_coeff   6   harmonic     1.9992000      110.33000
```

```
# Methylammonium
#@ H4 - N4 - C16
angle_coeff   7   harmonic     3.1083500      106.11000
#@ H4 - N4 - H4
angle_coeff   8   harmonic     1.6219500      105.67000
#@ N4 - C16 - H16
angle_coeff   9   harmonic     1.5303500      111.73000
#@ H16 - C16 - H16
angle_coeff  10   harmonic     1.7250000      116.28000

# Glycine (ZT)
#@ C18 - C17 - N5
angle_coeff  11   harmonic     1.5441000      114.70000
#@ C17 - N5 - H5
angle_coeff  12   harmonic     3.1083500      106.11000
#@ O18 - C18 - C17
angle_coeff  13   harmonic     2.8160500      115.04000
#@ O18 - C18 - O18
angle_coeff  14   harmonic     5.0780000      129.92000
#@ H5 - N5 - H5
angle_coeff  15   harmonic     1.6219500      105.67000
#@ H17 - C17 - N5
angle_coeff  16   harmonic     1.5303500      111.73000
#@ C18 - C17 - H17
angle_coeff  17   harmonic     1.9992000      109.26000
#@ H17 - C17 - H17
angle_coeff  18   harmonic     1.5441000      108.70000

################################################################################################
#### Covalent dihedral parameters
################################################################################################
#@ 7 dihedral types

dihedral_style charmm
#@  H14 - C14 - C15 - O15
dihedral_coeff   1        0.00005403   6   180   0.00000
#@ H4 - N4 - C16 - H16
dihedral_coeff   2        0.00703640   3   360   0.00000
#@ C18 - C17 - N5 - H5
dihedral_coeff   3        0.00703640   3   360   0.00000
#@ O18 - C18 - C17 - N5
dihedral_coeff   4        0.00005403   6   180   0.00000
#@ H17 - C17 - C18 - O18
dihedral_coeff   5        0.00005403   6   180   0.00000
#@ H5 - N5 - C17 - C18
dihedral_coeff   6        0.00703640   3   360   0.00000
#@ H5 - N5 - C17 - H17
dihedral_coeff   7        0.00703640   3   360   0.00000

################################################################################################
#### Covalent improper dihedral parameters
################################################################################################
#@  3   improper types

improper_style distance
#@  C4 - O4 - O4 - O4
improper_coeff   1     13.647000      360.00000

# Acetate
#@  C15 - C14 - O15 - O15
improper_coeff   2     8.3587000      360.00000

# Glycine (ZT)
#@ C18 - C17 - O18 - O18
improper_coeff   3     8.35870000     360.0000

################################################################################################
# Pair potentials
################################################################################################

variable rmin  equal 6.
variable rmax  equal 9.
variable rcoul equal 9.

pair_style hybrid/overlay coul/long ${rcoul}        &
                          lj/cut ${rmax}         &
lj/cut/soft 1.0 0.5 10.     &
                           lj/mdf ${rmin} ${rmax} &
                       lennard/mdf ${rmin} ${rmax} &
                          buck/mdf ${rmin} ${rmax}

pair_coeff       *       *             coul/long

################################################################################################
# Interactions with water
# Water - SPC/Fw
pair_coeff     ${O2}   ${O2}             lj/cut      0.00674        3.165492
pair_modify tail yes

# Alkaline metals
pair_coeff     ${Na}   ${O2}             lj/mdf      0.00012        3.738298
pair_coeff     ${K}    ${O2}             lj/mdf      0.015          3.15
pair_coeff     ${Rb}   ${O2}             lj/mdf      0.015          3.27
pair_coeff     ${Cl}   ${O2}             lj/mdf      0.022636       3.51

# Alkaline earths
pair_coeff     ${Mg}   ${O2}             lj/mdf      0.001137       2.82
pair_coeff     ${Ca}   ${O2}             lj/mdf      0.00095        3.35
pair_coeff     ${Sr}   ${O2}             lj/mdf      0.000776       3.65
pair_coeff     ${Ba}   ${O2}             lj/mdf      0.000657       3.965

# Carbonate
pair_coeff     ${O2}   ${O4}           buck/mdf  12534.455133       0.202          0.
pair_coeff     ${H2}   ${O4}           buck/mdf    340.             0.217          0.

# Acetate
pair_coeff     ${C14}  ${C14}            lj/mdf      0.0042100000   3.3611000000   6.0000   9.0000
pair_coeff     ${C14}  ${H14}            lj/mdf      0.0022700000   2.8244000000   6.0000   9.0000
pair_coeff     ${H14}  ${H14}            lj/mdf      0.0012300000   2.3734100000   6.0000   9.0000
pair_coeff     ${H14}  ${C15}            lj/mdf      0.0022700000   2.8244000000   6.0000   9.0000
pair_coeff     ${C15}  ${C15}            lj/mdf      0.0042100000   3.3611000000   6.0000   9.0000
```

```
pair_coeff     ${C14}  ${O15}            lj/mdf      0.0086700000   2.9708200000   6.0000   9.0000
pair_coeff     ${H14}  ${O15}            lj/mdf      0.0046800000   2.4964400000   6.0000   9.0000
pair_coeff     ${C15}  ${O15}            lj/mdf      0.0086700000   2.9708200000   6.0000   9.0000
pair_coeff     ${O15}  ${O15}            lj/mdf      0.0178800000   2.6258500000   6.0000   9.0000

# acetate - water
pair_coeff     ${O2}   ${O15}            lj/cut      0.0017955      3.27232
pair_coeff     ${O2}   ${O15}          buck/mdf   1105.             0.305          0.000
pair_coeff     ${O2}   ${C14}            lj/cut      0.00440        3.36693
pair_coeff     ${O2}   ${C15}            lj/cut      0.00440        3.36693
pair_coeff     ${O2}   ${H14}            lj/cut      0.00288        2.74099

# calcium - acetate
pair_coeff     ${Ca}   ${O15}          buck/mdf    2388.4841       0.271511        0.
pair_coeff     ${Ca}   ${C14}       lennard/mdf   12000.0000       0.0

# carbonate - acetate
pair_coeff     ${O4}   ${H14}       lennard/mdf      34.           0.0
pair_coeff     ${O4}   ${C15}          buck/mdf      67.475158     0.570000        0.

# Methylammonium
# lj/cut should have rmax=10
pair_coeff     ${O2}   ${C16}       lj/cut/soft       0.00440      3.36701         1.0
pair_coeff     ${O2}   ${H4}        lj/cut/soft       0.00000      1.00            1.0
pair_coeff     ${O2}   ${H16}       lj/cut/soft       0.00288      2.74105         1.0
pair_coeff     ${O2}   ${N4}        lj/cut/soft       0.00332      3.47115         1.0
pair_coeff     ${C16}  ${C16}       lj/mdf            0.00288      3.58118
pair_coeff     ${C16}  ${H4}        lj/mdf            0.00000      1.00
pair_coeff     ${C16}  ${H16}       lj/mdf            0.00188      2.91541
pair_coeff     ${C16}  ${N4}        lj/mdf            0.00437      3.35146
pair_coeff     ${H4}   ${H4}        lj/mdf            0.00000      1.00
pair_coeff     ${H4}   ${H16}       lj/mdf            0.00000      1.00
pair_coeff     ${H4}   ${N4}        lj/mdf            0.00000      1.00
pair_coeff     ${H16}  ${H16}       lj/mdf            0.00123      2.37341
pair_coeff     ${H16}  ${N4}        lj/mdf            0.00285      2.72839
pair_coeff     ${N4}   ${N4}        lj/mdf            0.00663      3.13647

# calcium - methylammonium
pair_coeff     ${Ca}   ${C16}       lennard/mdf    2724.137931     0.0

# carbonate - methylammonium
pair_coeff     ${O4}   ${H4}          buck/mdf     728.912480     0.250000        0.
pair_coeff     ${O4}   ${H16}       lennard/mdf    2750.           0.0

# bicarbonate - methylammonium
pair_coeff     ${O5}   ${H4}          buck/mdf     578.218500     0.250000        0.
pair_coeff     ${O5}   ${H16}       lennard/mdf    2181.470231     0.0
pair_coeff     ${O6}   ${H4}          buck/mdf     420.905395     0.250000        0.
pair_coeff     ${O6}   ${H16}       lennard/mdf    1587.968197     0.0

# Glycine (ZT)
pair_coeff     ${O2}   ${C17}        lj/cut/soft      0.00440      3.36701         1.0
pair_coeff     ${O2}   ${C18}        lj/cut/soft      0.00440      3.36701         1.0
pair_coeff     ${O2}   ${H5}         lj/cut/soft      0.00000      1.00000         1.0
pair_coeff     ${O2}   ${H17}        lj/cut/soft      0.00288      2.74105         1.0
pair_coeff     ${O2}   ${N5}         lj/cut/soft      0.00332      3.47115         1.0
pair_coeff     ${O2}   ${O18}        lj/cut/soft      0.00513      3.27240         1.0
pair_coeff     ${C17}  ${C17}            lj/mdf      0.00288      3.58118
pair_coeff     ${C17}  ${C18}            lj/mdf      0.00288      3.58118
pair_coeff     ${C17}  ${H5}             lj/mdf      0.00000      1.00
pair_coeff     ${C17}  ${H17}            lj/mdf      0.00188      2.91541
pair_coeff     ${C17}  ${N5}             lj/mdf      0.00437      3.35146
pair_coeff     ${C17}  ${O18}            lj/mdf      0.00717      3.06654
pair_coeff     ${C18}  ${C18}            lj/mdf      0.00288      3.58118
pair_coeff     ${C18}  ${H5}             lj/mdf      0.00000      1.00
pair_coeff     ${C18}  ${H17}            lj/mdf      0.00188      2.91541
pair_coeff     ${C18}  ${N5}             lj/mdf      0.00437      3.35146
pair_coeff     ${C18}  ${O18}            lj/mdf      0.00717      3.06654
pair_coeff     ${H5}   ${H5}             lj/mdf      0.00000      1.00
pair_coeff     ${H5}   ${H17}            lj/mdf      0.00000      1.00
pair_coeff     ${H5}   ${N5}             lj/mdf      0.00000      1.00
pair_coeff     ${H5}   ${O18}            lj/mdf      0.00000      1.00
pair_coeff     ${H17}  ${H17}            lj/mdf      0.00123      2.37341
pair_coeff     ${H17}  ${N5}             lj/mdf      0.00285      2.72839
pair_coeff     ${H17}  ${O18}            lj/mdf      0.00468      2.49644
pair_coeff     ${N5}   ${N5}             lj/mdf      0.00663      3.13647
pair_coeff     ${N5}   ${O18}            lj/mdf      0.00152      3.98580
pair_coeff     ${O18}  ${O18}            lj/mdf      0.01788      2.62585

# calcium - glycine (ZT)
pair_coeff     ${Ca}   ${O18}          buck/mdf    2388.4841       0.271511        0.
pair_coeff     ${Ca}   ${N5}           buck/mdf   22878.8          0.215023        0.
pair_coeff     ${Ca}   ${C17}       lennard/mdf   12000.0000       0.0
pair_coeff     ${O4}   ${H5}          buck/mdf     719.5374       0.250000        0.
pair_coeff     ${O4}   ${H17}       lennard/mdf     43.5625       0.0
pair_coeff     ${O4}   ${C18}         buck/mdf      53.9625       0.570000        0.

#########################################################################################
# Interactions with carbonate
pair_coeff     ${Mg}   ${O4}          buck/mdf    3944.8613        0.238160       0.

pair_coeff     ${Ca}   ${O4}          buck/mdf    3161.6335        0.271511       0.

pair_coeff     ${Sr}   ${O4}          buck/mdf   14250.2690        0.244116       0.

pair_coeff     ${Ba}   ${O4}          buck/mdf   13478.1510        0.258299       0.

pair_coeff     ${Na}   ${O4}          buck/mdf     689.21763       0.315407       0.

pair_coeff     ${Rb}   ${O4}          buck/mdf    2321.4110        0.299028       0.

special_bonds lj 0. 0. 0.5  coul 0. 0. 1.
```