# Modifying Lennard-Jones Parameters in the Amberff14SB force field

#### In this tutorial you will learn to:

- Modify the self-interaction Lennard-Jones parameters of oxygens of carboxylate groups in proteins.
- Modify the Lennard-Jones parameters defining the interaction between sodium ions and the oxygens of carboxylate groups in proteins.

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### Introduction

• The Amber formulation of the 6-12 Lennard-Jones (LJ) potential, V<sub>ii</sub>, between 2 atoms *i* and *j* is:

$$V_{i,j} = \varepsilon_{i,j} \left( \left( \frac{R_{\min,i,j}}{r_{i,j}} \right)^{12} - 2 \left( \frac{R_{\min,i,j}}{r_{i,j}} \right)^{6} \right)$$
 (eq. 1)

- Here  $R_{min,i,i}$  is the center-to-center distance between *i* and *j* at which the potential is at the minimum  $\varepsilon_{i,i}$ .
- Van der Waals data in Amber force field files are given for each atom *i* as a single data pair: a radius R<sub>min,i,i</sub>/2 ('van der Waals' radius of atom *i*, in Å) and the energy ε<sub>i,i</sub> (the minimum interaction energy between 2 atoms *i*, in kcal/mol). These parameters are also called the self-interaction parameters.
- For Amber force fields, cross terms involving different atom types *i* and *j* are typically evaluated according to the Lorentz/Berthelot mixing rules:

- In the first part of this tutorial you will learn how to modify self-interaction LJ parameters, using as example the parameters for the oxygens of carboxylate groups in proteins. Notice that, by modifying the self-interaction parameters of these oxygens, you are in fact modifying the LJ interactions of *every atom type with these oxygens*, via the mixing rules given by eqs. 2,3.
- The mixing rules have been shown to poorly represent the van der Waals interactions in certain cases. In the second part of this tutorial you will learn how to override the mixing rules for specific pairs of atoms *i* and *j*, and to use instead values of R<sub>min,i,j</sub> and/or ε<sub>ij</sub> optimized for that interaction. Specifically, you will modify the LJ parameters for the interaction between Na<sup>+</sup> and the oxygens in the carboxylate groups of proteins.
- The new parameters are from Kashefolgheta, S. & Vila Verde, A. PCCP, 2017, 19, 20593-20607, doi: 10.1039/ C7CP02557B. They yield better agreement with experiment for the hydration free energy of acetate and the solution activity derivative of 0.5 m sodium acetate in TIP3P water. The same paper also reports optimized parameters for the NH<sub>3</sub><sup>+</sup> group of lysine, which we recommend using to obtain a better description of salt bridges in proteins.

- The original parameter files for the AMBER force field are in a directory which in our system can be found via environmental variable \$AMBERHOME. The path to this directory is specific to each installation. If \$AMBERHOME is not defined in your system and you don't know the path, you will need to ask your local IT support for help. You will leave the original files unchanged, and you will do modifications on local copies.
- Create a directory Tutorial/ at a location of your choice. Copy the necessary files from \$AMBERHOME to Tutorial/ using the commands shown in fig. A.

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<pre>leaprc.DNA.bsc1</pre>	leaprc.GLYCAM 06EPb	leaprc.protein.fb15	leaprc.RNA.OL3
leaprc.DNA.OL15	leaprc.GLYCAM_06j-1	leaprc.protein.ff03.r1	leaprc.RNA.ROC
leaprc.ff14SB.redq	leaprc.lipid14	leaprc.protein.ff03ua	leaprc.RNA.YIL
leaprc.ffAM1	leaprc.lipid17	leaprc.protein.ff14SB	leaprc.water.fb3
leaprc.ffPM3	leaprc.modrna08	<pre>leaprc.protein.ff14SBonlysc</pre>	leaprc.water.fb4
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[geraili@hot cmd]\$	cp leaprc.water.tip3p	/usr/data/bgfs1/geraili/Simu	lation_area/Tutorial/
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• Once this step is complete, your Tutorial/ directory should have the files shown in Fig. B.



Fig. B: content of Tutorial/

• Copy the remaining necessary files following the commands in Fig. C.

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frcmod.chi0L4	frcmod.ions1lm_iod	frcmod.phmd	lipid11.dat
frcmod.conste	frcmod.ions234lm_1264_spce	frcmod.phosaa10	lipid14.dat
frcmod.constph	frcmod.ions234lm_1264_tip3p	frcmod.pol3	lipid17.dat
frcmod.dc4	frcmod.ions234lm_1264_tip4pew	<pre>frcmod.protonated_nucleic</pre>	lj_1264_pol.dat
frcmod.DNA.OL15	frcmod.ions234lm_126_spce	frcmod.qspcfw	music.dat
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frcmod.ff99SBnmr	frcmod.ionsjc_tip3p	frcmod.tip4pfb	parm96.dat
frcmod.ff99SP	frcmod.ionsjc_tip4pew	frcmod.tip5p	parm98.dat
frcmod.ions1lm_1264_spce	frcmod.meoh	frcmod.urea	parm99.dat
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frcmod.ions1lm_126_hfe_opc	frcmod.opc3	gaff2.dat	parmPM3.dat
frcmod.ions1lm_126_iod_opc	frcmod.parmbsc0	gaff.dat	toyrna.dat
frcmod.ions1lm_126_spce	frcmod.parmbsc0_ez0L1	GLYCAM_06EPb.dat	<pre>validate_torsions.py</pre>
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[geraili@hot parm]\$ cp frcmo@	d.ff14SB /usr/data/bgfs1/gerail	i/Simulation_area/Tutorial/	
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[geraili@hot lib]\$ <u>cp</u> aminon1	t12.lib /usr/data/bgfs1/geraili	/Simulation_area/Tutorial/	
[geraili@hot lib]\$			

- Once you've copied all the files, Tutorial/ should have the content shown in Fig. D.
- The files *leaprc.water.tip3p* and *leaprc.protein.ff14SB* are loaded into "tleap" to build topology and coordination files for simulations of proteins in water. These files contain, among other things:
  - a list of atom types;
  - the path to the parameter files that will be loaded by "tleap":
    - *leaprc.protein.ff14SB* calls parameter files *parm10.dat* and *frcmod.ff14SB* and topology files *amino12.lib, aminoct12.lib, aminont12.lib;*
    - *leaprc.water.tip3p* calls several parameter and topology files for TIP3P water and TIP3P-compatible ions; one of the files called is *frcmod.ionsjc\_tip3p*, which we have copied. We will not change anything in *leaprc.water.tip3p* or in *frcmod.ionsjc\_tip3*. We copied these files because 1) we want to view the original Na+ parameters for the second part of the tutorial, and 2) it is convenient to have in a single directory all the files necessary to run a simulation in the AMBER MD software.
- Now that we have all the files necessary, we need to modify them one by one. You will only modify files inside Tutorial/.

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amino12.lib	aminoct12.lib	aminont12.lib	frcmod.ionsjc_tip
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Fig. D: content of Tutorial/

- Our first, and most complex, task is to modify the self-interaction parameters of the oxygens in the carboxylate groups of proteins. Carboxylates exist in side chain of Asp (Asparate) and Glu (Glutamate) residues, and in any uncapped amino acid forming the C-terminus of the protein.
- In general, the difficulty in creating new atom types for a specific functional group is to make sure that we change the parameters of only the atom type on those functional groups, while leaving oxygens with the same original atom type but not belonging to the same functional group with the original parameters. In our specific example this problem does not arise because we only have these type of oxygens on the carboxylates in the side chain of Asp (aspartate) and Glu (glutamate) residues, and in any uncapped amino acid forming the C-terminus of the protein. We nevertheless follow a standard procedure to create a general tutorial for any other kind of optimization that might need to consider this important point.

• Open file *amino12.lib* with your favorite text editor and go to the entry for aspartate ("ASP"). The carboxylate oxygen has type "O2". An example section of the unmodified version of this file is in Fig. E.; the red boxes show you the lines containing "O2" for ASP.



Fig. E: original *amino12.lib* 

- In *amino12.lib*, change the atom type of the oxygens in the side chain of ASP from "O2" to a new type; we chose "90". • See Fig. F for the modified entries for ASP.
  - It is indispensable that the new atom type: 1) has only 2 letters; 2) is not already used for other atoms. You can check whether your new atom type is not being used by searching through this file.
- Search through this file and double check that atom type "O2" is changed to "9O" for every entry for ASP. Repeat the • procedure for glutamate ("GLU"). Save and close the file when you are done.



Fig. F: modified amino12.lib

- Amino acids forming the C- or N-terminus of a protein have separate entries in the AMBER force field. The C-terminus entries are in file *aminoct12.lib*; the N-terminus entries are in file *aminort12.lib*. You will need to modify these files as well.
- An example section of the unmodified version of *aminoct12.lib* is shown in Fig. G. Notice that you now have 2 carboxylates for CGLU (red boxes): one in the side-chain and one forming the C-terminus.



Fig. G: original aminoct12.lib

#### For the C-terminus (*aminoct12.lib*): ٠

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- Search for CGLU and change atom type "O2" to "9O", similarly to what you did before. Fig H shows an example section of the modified aminoct12.lib.

- Repeat for CASP.	emacs@lbox157.mpikg.mpg.de File Edit Options Buffers Tools Help	+ - @ ×
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carboxylate group; you	"H" "H" 0 1 131072 2 1 0.305500	
will need to change "O2"	"CA" "CX" 0 1 131072 3 6 -0.205900 "HA" "H1" 0 1 131072 4 1 0.139900	
to "90" for all those	"CB" "2C" 0 1 131072 5 6 0.007100 "HB2" "HC" 0 1 131072 6 1 -0.007800	
carboxylates too (examples	"HB3" "HC" 0 1 131072 7 1 -0.007800	
not shown).	"HG2" "HC" 0 1 131072 9 1 -0.054800	
- Save and close the file	"HG3" "HC" 0 1 131072 10 1 -0.054800 "CD" "CO" 0 1 131072 11 6 0.818300	
when you are done.	"0E1" "90" 0 1 131072 12 8 -0.822000 "0E2" "90" 0 1 131072 13 8 -0 822000	
	"C" "C" 0 1 131072 14 6 0.742000	
For the N-terminus	"0XT" "90' 0 1 131072 16 8 -0.793000	
(aminont12.11b):	<pre>!entry.cgLU.unit.atomspertinfo table str pname str ptype int ptypex int pelmnt dbl pchg     "N" "N" 0 -1 0.0</pre>	
- Repeat the procedure to	"H" "H" 0 -1 0.0	
modify the side-chain	"HA" "H1" 0 -1 0.0	
oxygens in NASP and	"CB" "2C" 0 -1 0.0 "HB2" "HC" 0 -1 0.0	
NGLU (images not shown).	"HB3" "HC" 0 -1 0.0 "CG" "2C" 0 -1 0.0	
Only these amino acids	"HG2" "HC" 0 -1 0.0	
need to be modified in this	"HG3" "HC" 0 -1 0.0 "CD" " <u>C0"</u> 0 -1 0.0	
file, because N-terminus	"0E1" "90' 0 -1 0.0 "0E2" "90' 0 -1 0.0	
amino acids do not contain		
extra carboxylate groups.	"0XT" "90' 0 -1 0.0	
- Save and close the file	!entry.CGLU.unit.boundbox array dbl -1.000000	
when you are done.		
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Fig. H: modified section of *aminoct12.lib* 

- In the *leaprc.protein.ff14SB* file, copy the line where "O2" is defined (green box in Fig. I), and paste it directly below it as a new line.
- In the new line, change the "O2" to "YOUR NEW NAME" (in our example, the new name is "90"; red box in Fig. I).
- Save and close the file.

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{ "CH" "C" "sp3" }		
{ "CS" "C" "sp2" }		
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{ "CO" "C" "sp2" }		
{ "C*" "C" "sp2" }		
-: leaprc.protein.ff14SB 4% L23 (Fundamental +2)		

- The actual parameter values atomic masses, charges, Lennard-Jones, bonds, angles, dihedral and improper potentials for each interaction between 2 or more atoms are in files *parm10.dat* and *frcmod.ff14SB*.
  - *parm10.dat* is the main file; it contains the parameters for most interactions, and it is **never** modified.
  - *frcmod.ff14SB* supplements *parm10.dat* in two different ways: 1) it contains parameters for any new interaction;
     2) it may also contain new parameters for any interaction that is already defined in *parm10.dat* but which we wish to override.
    - "tleap" reads *parm10.dat* first and *frcmod.ff14SB* afterwards; if it finds parameters for the same interaction in both files, it will use those from *frcmod.ff14SB* only.
  - In the next few slides we will illustrate the procedure to include in *frcmod.ff14SB* parameters for all interactions involving our new atom type "9O". In general, the steps in the procedure are (do not worry if you do not understand the procedure at this point; the examples will clarify it):
    - step 1: for each reference to carboxylate-"O2" in *parm10.dat*, check if the same interaction has been defined in *frcmod.ff14SB*.
      - If yes, duplicate the line in *frcmod.ff14SB* and past the duplicate directly below the original line; in the duplicate line, change "O2" to "9O".
      - if no, copy the line in *parm10.dat*, paste it at the end of the corresponding section in *frcmod.ff14SB*; in the copy, change "O2" to "9O".
      - by following these instructions, you make sure that all parameters in *parm10.dat* for carboxylate-"O2" are put into *frcmod.ff14SB*, without overwriting newer parameters for the same interaction if they exist in *frcmod.ff14SB*.
    - step 2: once you're done with step 1, you need to search for all references to carboxylate-"O2" in *frcmod.ff14SB*, and make sure that equivalent information is defined for "9O". This step is necessary because some interactions may only be defined in *frcmod.ff14SB*.

- Entering mass information for "90":
  - Look for the mass of "O2" in *parm10.dat* (Fig. J, red box).
  - Inspect the MASS section in *frcmod.ff14SB*. There is no entry for "O2" there.
    - Copy the line containing the mass information from *parm10.dat*, paste it at the end of the MASS section in *frcmod.ff14SB* and change the atom type from O2 to "9O" (Fig. K, red box).

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C8-CX	310.0	1.5260	
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C8-HC	340.0	1.0900	
C8-HP	340.0	1.0900	
C8-N2	337.0	1.4630	
C8-N3	367.0	1.4710	
CA-2C	317.0	1.5100	
CC-2C	317.0	1.5040	

Fig. K: modified section of *frcmod.ff14SB* 

Fig. J: Original parm10.dat

- Entering parameters for bonds involving "90":
  - locate bond parameters involving "O2" in *parm10.dat*. Here is the relevant line:
    - C -O2 656.0 1.250 JCC,7,(1986),230; GLU,ASP (line 81)
    - O2-P 525.0 1.480 JCC,7,(1986),230; NA PHOSPHATES (line 173)
  - locate bond parameters involving "O2" in *frcmod.ff14SB*. There is only one line:
    - CO-O2 656.0 1.2500

- (line 20)
- Interactions "C –O2" and "O2-P" are only defined in *parm10.dat*. Copy the line for "C –O2" from *parm10.dat*, paste it at the end of the bond section in *frcmod.ff14SB* and change "O2" to "9O" (Fig. L, green box).
  - Note that you should **not** insert a line for the "9O-P" bond in *frcmod.ff14SB*. We developed these oxygen parameters specifically for carboxylates. Because of their high specificity, these parameters should not be used for anything other than the intended functional groups.
- Interaction "CO-O2" only exists in *frcmod.ff14SB*. Duplicate this line, past it directly below the original and change "O2" to "9O" (Fig. L, red box).
  - Note: if "CO-O2" had simultaneously existed in *parm10.dat*, you would have ignored the *parm10.dat* data and would have done exactly the same.

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r	C8-	68	310.0		1.520	60															
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	HC -	3C	340.0		1.090	00															
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Fig. L: modified section of *frcmod.ff14SB* 

- Entering parameters for angles, dihedrals or impropers involving carboxylate-"O2":
  - To make these changes, you follow the same procedure we have exemplified for inserting parameters for bonds involving "9O", with one difference: when you are changing the carboxylate-"O2" angle, dihedral, or improper, you must change them in a way to be able to consider any combination of interactions in the future.
    - search for carboxylate angles with "O2" in *parm10.dat*. There are multiple lines:

—	CT-C -O2	70.0	117.00			(line 237)
-	CX-C -O2	70.0	117.00	(was CT-C	-O2)	(line 238)
-	02-C -02	80.0	126.00	AA GLU	(SCH JPC 79,2379)	(line 254)
-	02-P -OH	45.0	108.23			(line 539)
_	02-P -02	140.0	119.90			(line 540)
_	02-P -0S	100.0	108.23			(line 543)

- do the same thing in *frcmod.ff14SB*. Here are the lines:
  - O2-CO-O2 80.0 126.00
  - O2-CO-2C 70.0 117.00
- Notice that each angle interaction is defined in only one file.
- Duplicate the line with the "O2-CO-2C " interaction in *frcmod.ff14SB* and paste it directly below the original. In the duplicate, change "O2" to "9O" (green box in Fig. M)
- Duplicate the line with the "O2-CO-O2" interaction in *frcmod.ff14SB* and paste it twice directly below the original. In the duplicates, change "O2" to "9O" to allow all possible combinations of "O2" and "9O" (red box in Fig. M)
  - For our specific application, it would have been sufficient to insert only a line with "9O-CO-9O" in *frcmod.ff14SB* because the \*lib files we modified do not have an "O2-CO-O9" angle. We nevertheless suggest always including the combinations in *frcmod.ff14SB* to avoid unexpected problems if an angle "9O-CO-O2" ever becomes necessary.
- Copy each of the lines from *parm10.dat* with angle interactions involving carboxlyate-"O2" and paste them one or more times (as necessary) at the end of the ANGLE section in *frcmod.ff14SB*. Make the necessary changes from "O2" to "9O" (images not shown).
- Angle potentials involving the "O2-P" bond (in red above) should **not** be updated to "9O" in *frcmod.ff14SB*, for the reasons explained in the previous slide.
- Follow the same procedure to update dihedral and impropers (images not shown).

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I	02-	C0-	90	80.	0	126.00	new	par	amet	er
I	02-	CU-	2C	70.	0	117.00				
I	90-	C0-	2C	70.	0	117.00	new	par	amet	er
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- We will now input the new Lennard-Jones (LJ) parameters for atom type "90". LJ parameters exist in *parm10.dat* (Fig. N; red box shows parameters for "O2"), and in *fremod.ff14SB*, in the "NONB" and "LJEDIT" sections (Fig. O, red boxes).
  - The "NONB" section will contain the new self-interaction parameters.
  - the "LJEDIT" will contain LJ parameters for those pairs of atoms for which we want to override the Lorentz-Berthelot combination rules.

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• Download the \*zip file that you'll find as supporting information of the article we mentioned in the introduction (doi: 10.1039/C7CP02557B). Open file Parameters/Acetate.top. This file contains the LJ parameter information in gromacs format; amber format parameters are given as comments. The relevant lines for this tutorial are:

Rij(AMBER; A) epsilon ij(AMBER, kcal/mol)

-	;name	bond_type	mass	charge	ptype	sigma (nm)	epsilon (kJ/mol)	)	r(AMBER; A)	epsilon	(AM	BER; kcal/mol)
-	OACE	OACE	0.00000	0.0000	) A	2.95992e-01	6.76553e-01	;	1.6612	0.1617	;	0.77x Original epsilon

epsilon

- OACE NA+ 1 2.75899e-1 4.97508e-1 ; 3.0969

sigma

0.1189 ; 1.022 times Original sigma (Rij in AMBER) ;

OACE self iteraction correction for epsilon included

"OACE" corresponds to our "90". "r(AMBER)" and "epsilon (AMBER)" are the optimized self-interaction parameters. "r(AMBER)" is  $R_{min,i,i}/2$  and "epsilon(AMBER)" is  $\epsilon_{i,i}$  in the notation of eq. 1 of this tutorial.

func

:i

i

- "Rij(AMBER)" and "epsilon\_ij(AMBER)" are the optimized LJ parameters for the interaction between "O9" and Na<sup>+</sup>. Notice that "Rij(AMBER)" is R<sub>min,i,j</sub> in the notation of eq. 1.
- Notice that "r(AMBER)" is the same as in *parm10.dat* (Fig. N) but that "epsilon (AMBER)" is different: the optimized "r(AMBER)" is 0.77 times the original "r(AMBER)".
- Insert the new LJ self-interaction parameters ("r(AMBER)" and "epsilon (AMBER)") for "90" into *frcmod.ff14SB* as shown in Fig. P.

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N3-CX-2C-S	1 0	.469	Θ.Θ	1.				
CX-2C-S -S	1 0	. 135	180.0	-4.				
CX-2C-S -S	1 0	.302	Θ.Θ	-3.				
CX-2C-S -S	1 0	.666	0.0	-2.				
CX-2C-S -S	1 0	.056	Θ.Θ	1.				
2C-S -S -2C	1 0	.379	0.0	-4.				
2C-S -S -2C	1 0	.682	Θ.Θ	-3.				
2C-S -S -2C	1 4	.480	0.0	-2.				
2C-S -S -2C	1 0	.420	Θ.Θ	1.				
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X -02-C0-02	1	0.5	180.	2.				
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C	1 0000	0.109		Spellmover				
co	1.9080	0.1094	•	opic				
00	1.9080	0.0860	7	DCCD 2017	10 20502			
90	1.6612	0.161	/	PCCP, 2017,	19, 20593			

Fig. P: modified frcmod.ff14SB

- Now for the second (and shorter) part of this tutorial: modifying the LJ interactions between "90" and Na<sup>+</sup>:
- We will start by examining the original ion parameters (from JPCB 2008, 112, 9020-9041) typically used with TIP3P water. Open file Tutorial/*frcmod.ionsjc\_tip3p*. The values under the NONBON section are  $R_{min,i,i}/2$  (in A) and  $\varepsilon_{i,i}$  (in kcal/mol). This file is loaded in "tleap" following the indications in *leaprc.water.tip3p*; to confirm this information, open *leaprc.water.tip3p* and search for the text string "frcmod.ionsjc\_tip3p".

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Cl- 35.45		1.9	910			(	chlor	ine	(Appl	.eqı	iis	t)
Br- 79.90		2.8	880				bromi	ne	(Appl	.eqı	iis	t)
I- 126.9		4.0	690			:	iodin	e	(Appl	.eqı	iis	t)
NONBON												
Li+	1.025	(	0.027	9896								
Na+	1.369	(	0.087	4393								
K+	1.705	(	0.193	6829								
Rb+	1.813	(	0.327	8219								
Cs+	1.976	(	0.406	5394								
F-	2.303	(	0.003	3640								
	2.513		0.035	5910								
Br-	2.608		0.058	6554								
1-	2.860		0.053	6816								
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Fig. Q: original *frcmod.ionsjc\_tip3p* 

- Entries in the "LJEDIT" section in *frcmod.ff14SB* have the following (unexpected!) format:
  - atom\_type\_A atom\_type\_B  $d_A = E_A = d_B = \frac{1}{2}$ ; "d" in angstrom; E in kcal/mol
  - these parameters are *exclusively* used to define the interactions between atom type A and atom type B as

$$R_{\min,A,B} = d_A + d_B \qquad \qquad \varepsilon_{A,B} = \sqrt{E_A E_B}$$

- Notice that *any* combination of  $d_A$  and  $d_B$ , and of  $E_A$  and  $E_B$ , that yields the correct values  $R_{\min,A,B}$  and  $\varepsilon_{A,B}$  is allowed.  $d_A, E_A$  and  $e_B, E_B$  are, by themselves, meaningless; only  $R_{\min,A,B}$  and  $\varepsilon_{A,B}$  have meaning.
- In the "LJEDIT" section of *frcmod.ff14SB*, add the new parameters for the "90"..."Na+" interaction (red box, Fig. R).
- Notice that you could have also written:
   90 Na+ 1.54845 0.1189 1.54845 0.1189
   or
   90 Na+ 0 1 3.0969 0.01414
   where 0.01414=0.1189\*0.1189

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- Save and close *frcmod*.*ff14SB* when you are done.

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CA-CA-CA-2C	1.1	180.	2.				
NONB							
2C	1.9080 0.109	4	Spellmeyer				
3C	1.9080 0.109	4	Spellmeyer				
C8	1.9080 0.109	4	Spellmeyer				
CO	1.9080 0.086	0	0PLS				
90	1.6612 0.161	/	PCCP, 2017,	19, 20593			
LJEDIT							
90 Na+	3.0969 0.11	89 0 0.118	9				

- The final step is to update the paths to your modified parameter and topology files so they are loaded by "tleap".
  - Open Tutorial/*leaprc.protein.ff14SB* and update the paths of *parm10.dat*, *frcmod.ff14SB*, amino12.lib, *aminoct12.lib* and *aminont12.lib* to your Tutorial/ directory, as exemplified in Fig. S. We did not modify *parm10.dat* but it is convenient to call it also from Tutorial/ rather than from \$AMBERHOME. Save and close *leaprc.protein.ff14SB* when you are done.
  - Create a new file (we called it *ff14\_tleap\_-f\_ThisName.in*; Fig T) and add the following command: source /your/path/to/Tutorial/leaprc.protein.ff14SB
    - if you had made modifications in any of the water files, you could also add the command:

source /your/path/to/Tutorial/leaprc.water.tip3p

- save and close *ff14\_tleap\_-f\_ThisName.in*.
- To build topology (.prmtop) and coordination (.inpcrd) files using the new parameters, open "tleap" with the following command:

\$ tleap -f "YOUR DIRECTORY"/ ff14\_tleap\_-f\_ThisName.in

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🕐 🖴 📓 🗶 🏥 Save 🥱 Undo 🖌 🖡 💼 🔍		<pre># sourcing the Amber protein ff14Sb and water tip3p</pre>	
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- It is always useful to verify if you've made the correct the modifications. To do so, download *wt1mg.pdb* from "ambermd.org" (<u>http://ambermd.org/tutorials/advanced/tutorial8/files/wt1mg.pdb</u>). This is a protein that has already been prepared for simulation. Put the pdb file in a "new\_folder".
- Go to "new\_folder", open a terminal there, and type all the commands in Fig. U (use your own path to Tutorial/, where you've saved all the modified topology and parameter files). After all the commands are executed, type "quit".





- Now we will use "Parmed" (<u>https://parmed.github.io/ParmEd/html/index.html</u>) to inspect the "mol.prmtop" topology file. Type the following commands in the terminal
  - \$ parmed -p mol.prmtop
    \$ printLJMatrix :ASP
    \$ printLJMatrix :Na+
  - The last column shows  $\varepsilon_{i,j}$  in kcal/mol; the second-from-last column shows  $R_{min,i,j}$  in angstrom.

Take a look at the self-interaction parameters involving "9O" (Fig. V, red box) and at the interaction parameters between "9O" and "Na+" (Fig. V, green box). Compare them with those in file acetate.top, and with the parameters for "O2". Make sure there are no mistakes.

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<pre>M, M2, M3, M4, M8 [1] 90 [14] 532490. 597000 594.258905 3.457200 0.165798 2C, 3C, CB, CT, CX [3] 90 [14] 900.209543 1.3.470034 2.261200 0.056385 2C, 3C, CB, CT, CX [3] 90 [14] 990.209543 1.3.470034 2.261200 0.056385 2C, 3C, CB, CT, CX [3] 90 [14] 990.444940 44.66639 3.559200 0.133004 H1 [5] 90 [14] 990.444940 44.66639 3.559200 0.0558385 C, C*, CA, CB, CC, CN, CO, CR, CV, CW [7] 90 [14] 141 32420.995100 88.841213 3.661200 0.958385 C, C*, CA, CB, CC, CN, CO, CR, CV, CW [7] 90 [14] 141 33340.107000 445.6551343 3.322400 0.11925 0.11925 0.11925 0.11925 0.1192 0.119 0.111 90 [14] 413380.00000 552.20000 0.049249 0.11925 0.00000 455.6272 3.070200 0.049249 0.11925 0.101 90 [14] 413366.00000 655.20000 0.049249 0.0141 90 [14] 41336.00000 6552.20000 0.049249 0.0141 90 [14] 90 [14] 97788.712000 0.849249 0.04000 0.049249 90 [14] 90 [14] 90 [14] 925584.273000 424.062208 3.322400 0.161700 90 [14] 90 [14] 90 [14] 229504.877000 434.062208 3.322400 0.049249 90 [14] 90 [14] 90 [14] 229504.877000 434.062208 3.322400 0.049424 90 [14] 90 [14] 90 [14] 22759.9000 82.541620 3.102000 0.949249 90 [14] 90 [14] 90 [14] 22759.9000 82.541620 3.102000 0.949249 90 [14] 90 [14] 90 [14] 92558.42300 299.785247 3.0005000 0.118090 90 [14] 90 [14] 912775.910000 0.049617 9.3002000 0.049617 90 [14] 94 91 92 10.00000 0.00000 0.00000 0.00000 0.118090 90 [14] 96 112 927594.8310 299.785247 3.005000 0.118090 90 [14] 96 [14] 9755.42300 299.785247 3.005000 0.118090 90 [14] 96 [14] 9755.42300 299.785247 3.005000 0.121921 90 [14] 96 [14] 9755.42300 290.785247 3.005000 0.118090 90 [14] 96 [14] 9755.42300 290.785247 3.005000 0.118090 90 [14] 96 [14] 9755.42300 290.785247 3.005000 0.121921 90 [14] 96 [14] 9755.42300 290.785247 3.005000 0.121921 90 [14] 96 [14] 9755.42300 290.785247 3.005000 0.121921 90 [14] 96 [14] 9755.42300 290.785247 3.005000 0.037651 90 [14] 96 [14] 9772.745000 2556.405223 3.3130000 0.121921 90 [14] 96 [14] 9755.42300 290.785247 3.006000 0.037651 90 [14] 96 [14] 9772.745000 2556.405203 3.777000 0.037651 90 [14] 96 [14] 9772.745000 256.76</pre>	HC [11]	HW [20]	0.00000	0.00000	0.000000	0.00000	
H, HS [2]         90 [14]         900 [2059543         13.470834         2.261200         0.050385           2C, 3C, CB, CT, CX [3]         90 [14]         90664.44940         44.66333         2.761200         0.050385           HI [5]         90 [14]         9806.444940         44.66333         2.761200         0.050385           C, C*, CA, CB, CC, CN, CO, CR, CV, CW [7]         90 [14]         1564282.214000         486.793330         3.562200         0.17925           0         181         90 [14]         133340.187000         495.685439         3.322400         0.184274           0         181         90 [14]         13333.787000         95.223123         3.382200         0.184450           0         181         90 [14]         13333.787000         95.223123         3.382200         0.44450           H (11)         90 [14]         47758.712600         98.1937.13.44200         0.60235         0.44224           H (11)         90 [14]         47758.712600         98.1937.3.42200         0.60235           101         90 [14]         M2         24554.275000         28.49577.3.072200         0.646617           90 [14]         M2         24554.275000         249.75503         2.092766         0.172400         0.646617	N,N2,N3,NA,NB [1]	90 [14]	532490.587000	594.258905	3.485200	0.165798	
2C, 3C, CB, CT, CX [3] 90 [14] 566478.812000 540.944639 3.652208 0.133004 H1 [5] 90 [14] 9206.444940 44.66339 2.761208 0.050385 S, SH [6] 90 [14] 32420.95100 80.334282 3.0482208 0.050385 C, C*, CA, CB, CC, CN, CO, CR, CY, CV [7] 90 [14] 166229,750409 468.4319 3.56240 0.117925 0 [3] 90 [14] 33340.187000 469.63439 3.322408 0.148274 0 [19] 90 [14] 111 540428.214800 449.593318 3.56240 0.117925 0 [11] 90 [14] 41303 0707000 552.209132 3.382260 0.184274 0 [19] 90 [14] 41303 0707000 552.209132 3.382260 0.184274 0 [11] 90 [14] 47758,712600 98,108071 3.148208 0.050385 H4 [12] 90 [14] 47758,712600 98,108071 3.148208 0.050385 H4 [12] 90 [14] 47758,712600 98,108071 3.148208 0.050385 H4 [12] 90 [14] 47758,712600 882,495772 3.076200 0.049249 90 [14] 90 [14] 4192 22504 827000 882,495773 3.076200 0.049249 90 [14] 90 [14] 90 [14] 242504 827000 882,495773 3.076200 0.049249 90 [14] 90 [14] 90 [14] 242504 827000 882,495773 3.076200 0.049249 90 [14] 90 [14] 90 [14] 241596.423300 240.78524 3.322400 0.046517 90 [14] 90 [14] 90 [14] 90 [14] 92554 0.174200 0.075862 90 [14] 90 [14] 90 [14] 90 [14] 92596 0.05625 4.174200 0.075862 90 [14] 90 [14] 90 [14] 90 [14] 92596 0.05625 4.174200 0.075862 90 [14] 90 [14] 90 [14] 90 [14] 92596 0.05625 4.174200 0.075862 90 [14] 90 [14] 90 [14] 90 [14] 91 [15] 91 [16] 937000 91 [16] 9258 [16] 91 [16] 91 [16] 91 [16] 91 [16] 937000 91 [16] 90 [16] 90 [16] 91 [16] 91 [16] 91 [16] 937000 91 [16] 91 [16] 91 [16] 91 [16] 91 [16] 91 [16] 91 [16] 91 [16] 91 [16] 91 [16] 91 [16] 91 [16] 91 [16] 91 [16] 91 [16] 925 [16] 91 [16] 91 [16] 91 [16] 91 [16] 91 [16] 91 [16] 91 [16] 926 [16] 91 [16] 91 [16] 91 [16] 91 [16] 91 [16] 90 [16] 91 [1	H,HS [2]	90 [14]	900.269543	13.470034	2.261200	0.050385	
HP       [4]       90       [14]       9806       444940       44.666339       2.761260       0.050385         K       S, SH       [6]       90       [14]       1166289       750800       966.491310       3.661280       0.201060         C, C*, CA, CB, CC, CN, CO, CR, CV, CW       [7]       90       [14]       33340.187000       495.685439       3.322400       0.144774         H0       [10]       90       [14]       433303.767000       955.20123       3.322400       0.144450         H0       [10]       90       [14]       433303.767000       95.18213       3.322400       0.144450         H0       [10]       90       [14]       47758.71260       9.609213       3.422400       0.609285         H1       [12]       90       [14]       47758.71260       9.62310       3.422400       0.60385         H1       [12]       90       [14]       47758.71260       9.672143       3.072400       0.643249         H1       [12]       90       [14]       41236       7.43080       7.44749       0.72268       0.64617         H0       [14]       Max       [16]       292555.428100       243.452245       3.322460       0.64	2C,3C,C8,CT,CX [3]	90 [14]	568478.812000	549.944639	3.569200	0.133004	
H [5] 90 [14] 32420.995100 80.834/82 3.048200 0.050385 S,SH [6] 90 [14] 1166289.750000 908.401319 3.661200 0.201060 C,C*,CA,CB,CC,CN,CO,CR,CV,CW [7] 90 [14] 504080 495.568439 3.322400 0.184274 0H [9] 90 [14] 4133340.870000 552.209132 3.382200 0.184274 0H [9] 90 [14] 41303.070000 552.209132 3.382200 0.184274 0H [9] 90 [14] 4130.070000 6.000000 0.000000 0.000000 HC [11] 90 [14] 47758.712600 98.108971 3.148200 0.650385 H4 [12] 90 [14] 43546.229008 82.495572 3.070200 0.049249 00 [14] 90 [14] 427594.877000 434.962208 3.322400 0.649249 00 [14] 90 [14] 429254.877000 434.962208 3.322400 0.649249 00 [14] 90 [14] 4292544.877000 434.962208 3.322400 0.649249 90 [14] M22+ [16] 23488.714906 61.774949 3.021200 0.049249 90 [14] M22+ [16] 23488.714906 61.774949 3.021200 0.049249 90 [14] M22+ [16] 23488.714906 61.774949 3.021200 0.049617 90 [14] M22+ [16] 23488.714906 61.774949 3.021200 0.049617 90 [14] M22+ [16] 23488.714906 61.774949 3.021200 0.049617 90 [14] M22+ [16] 1.92535.428300 209.785247 3.085900 0.189900 90 [14] M22+ [16] 1.92535.428300 209.785247 3.195000 0.000000 9.000000 0.000000 0.000000 0.000000 0.000000	HP [4]	90 [14]	9896.444940	44.660339	2.761200	0.050385	
<pre>c, c+, cA, CB, CC, (N, CO, CR, CV, CW [7] 90 [14] 1166299 750000 968.491319 3.661200 0.201060 C, C+, CA, CB, CC, (N, CO, CR, CV, CW [7] 90 [14] 504028.214000 447 595330 3.559200 0.117925 H0 [10] 90 [14] 413333.707060 552.209132 3.322400 0.184456 H0 [10] 90 [14] 413333.707060 552.209132 3.322400 0.069000 HC [11] 90 [14] 47758.712600 98.108971 3.148200 0.069000 H4 [12] 90 [14] 41936.27900 90.201203 0.069030 H4 [12] 90 [14] 41936.27900 90.201203 0.069030 H4 [12] 90 [14] 41936.27900 90.201203 0.069030 H4 [12] 90 [14] 41936.27900 90.20120 0.049249 90 [14] 90 [14] 41936.27900 90.20120 0.049249 90 [14] 90 [14] 292540.877000 434.962208 3.322400 0.049249 90 [14] 90 [14] 222540.877000 61.775573 3.027000 0.049249 90 [14] M2 + [15] 28368.023500 74.755793 3.027000 0.049249 90 [14] M2 + [16] 234387.14900 61.774549 3.027200 0.0496417 90 [14] Ma + [18] 92535.428300 720.785427 3.0969000 0.118900 0.069000 0.069000 0.069000 0.069000 0.069000 0.069000 &gt; printLJMatrix :Na+ A tom Type 1 Atom Type 2 A coefficient B coefficient R 1,1 Eps 1,1 N,N2,N3,MA,NB [1] Na+ [18] 136919.347000 258.495233 3.193000 0.121921 H,H5 [2] Na+ [18] 1259.8270601 4.318247 1.969000 0.0715057 90 [14] HW [20] 0.000000 0.069000 0.0697005 HP [4] Na+ [18] 13991.347000 252.422368 3.277000 0.037051 C, C+, CA, CB, CC, CN, CO, CR, CV, CW [7] Na+ [18] 136197.919000 432.237832 3.359000 0.121921 H1 [5] Na+ [18] Na+ [18] 1316197.919000 432.237832 3.359000 0.0174551 C, C+, CA, CB, CC, CN, CO, CR, CV, CW [7] Na+ [18] 1316197.919000 422.242668 3.2771000 0.037051 HC [11] Na+ [18] 132910.267000 214.778698 3.2771000 0.037051 H1 [5] Na+ [18] 132910.267000 24.247268 3.2778000 0.037051 H1 [5] Na+ [18] 132910.267000 40.21472 2.856000 0.037051 H3 [18] Na+ [18] 0W [20] 0.000000 0.000000 0.000000 0.037051 H4 [12] Na+ [18] 000 [19] 104209 337.02960 22.778000 0.037551 Na+ [18] Na+ [18] 0W [20] 0.000000 0.000000 0.000000 0.037651 Na+ [18] 0W [19] 10420.861000 29.637570 3.137300 0.015266 Na+ [18] 0W [19] 10420.861000 0.9193777 3.137300 0.015266 <td>H1 [5]</td><td>90 [14]</td><td>32420.995100</td><td>80.834282</td><td>3.048200</td><td>0.050385</td></pre>	H1 [5]	90 [14]	32420.995100	80.834282	3.048200	0.050385	
C, C+, CA, CB, CC, CN, CO, CR, CV, (W [7] 90 [14] 50428.214060 487.595330 3.559200 0.117925 0 [8] 90 [14] 333340.117060 487.595.685439 3.322400 0.1844750 0H [9] 90 [14] 41333340.117060 495.52.20132 3.332200 0.184459 0H [11] 90 [14] 41333.707060 552.20132 3.332200 0.184459 HG [11] 90 [14] 41433.707060 95.108971 3.148200 0.060308 HG [11] 90 [14] 435456.220600 82.495572 3.070200 0.049249 90 [14] 90 [14] 4134546.220600 95.108971 3.148200 0.049249 90 [14] 90 [14] 4134546.220600 95.201912 3.120200 0.049249 90 [14] HS [15] 22886.023560 74.755793 3.020206 0.049249 90 [14] HS [15] 228486.714960 61.774494 3.120200 0.049249 90 [14] Mg2+ [16] 23488.714960 61.774949 3.120200 0.049249 90 [14] CL : 171 212275.910060 8802.591625 4.174206 0.045617 90 [14] 0.0411 Mg2+ [16] 23488.714960 60.2591625 4.174206 0.075662 90 [14] 0.0411 HW [20] 0.060060 0.0600600 0.18990 90 [14] 0.060060 0.0600600 0.18990 90 [14] 0.0113 41950.405066 5.16.142006 0.200060 0.121921 N,N2,N3,NA,NB [1] Na+ [18] 136019.347060 256.405233 3.193000 0.121921 N,N2,N3,NA,NB [1] Na+ [18] 136019.347060 256.405233 3.193000 0.2121921 N,N2,N3,NA,NB [1] Na+ [18] 136019.347060 256.405233 3.193000 0.02121921 N,N2,N3,NA,NB [1] Na+ [18] 13617.09006 42.242666 3.277000 0.097851 2C, 3C, 6, CT, CX [3] Na+ 181 13909.267860 2.373733 3.39000 0.037651 C, C+, CA, CB, CC, CN, CO, CR, CV (W [7] Na+ 118] 136197.90006 42.247666 3.277000 0.097851 C, C+, CA, CB, CC, CN, CO, CR, CV (W [7] Na+ 118] 136197.90000 42.247460 1.2778000 0.037651 HI [5] Na+ [18] 1001 Na+ [18] 131017.652760 2.2778000 0.037651 HI [5] Na+ [18] 1000 Na+ [18] 31211.662800 2.078050 0.037651 HI [5] Na+ [18] 1000 Na+ [18] 131000000 0.000000 0.037651 HI [13] Na+ [18] 000000 0.0381844565 3.882000 0.037651 HI [14] Na+ [18] 0072.727292 0.978534	S,SH [6]	90 [14]	1166289.750000	968.491319	3.661200	0.201060	
0 [8] 90 [14] 90 [14] 413303.70060 455.209132 3.322406 0.184474 H0 [10] 90 [14] 413303.70060 55.209132 3.322406 0.184450 H0 [11] 90 [14] 47756.712660 90.1089757 3.070200 0.090249 H4 [12] 90 [14] 3456.229060 82.495572 3.070200 0.049249 90 [14] 90 [14] 41936.27200 -0.091210 -3.120200 0.049249 90 [14] 90 [14] 41936.27200 -0.091210 -3.120200 0.049249 90 [14] H5 [15] 28368.02560 434.965208 3.322400 0.161700 90 [14] H6 [15] 28368.02560 434.965208 3.322400 0.049249 90 [14] H7 [2122775.91000 66] 5.91625 4.174200 0.049617 90 [14] H8 [15] 24388.714900 61.774949 3.021200 0.049617 90 [14] H8 [15] 414950.45060 5.10142006 0.342949 90 [14] H8 [13] 414950.45060 5.10142006 0.012975 90 [14] H8 [19] 414950.45060 5.10142006 0.010275 90 [14] H8 [19] 414950.45060 5.10142006 0.010275 90 [14] H8 [19] 414950.45060 5.10142006 0.010275 90 [14] H8 [20] 0.000000 0.000000 0.000000 0.000000 9.000000 0.000000 0.000000 0.000000 0.000000	C,C*,CA,CB,CC,CN,CO,CR,CV,CW [7]	90 [14]	504028.214000	487.595330	3.569200	0.117925	
$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$	0 [8]	90 [14]	333340.187000	495.685439	3.322400	0.184274	
H0       [16]       90       [14]       0.000000       0.000000       0.000000         H4       [12]       90       [14]       47758.712600       98.108971       3.142200       0.050305         H4       [12]       90       [14]       44956.27900       08.049572       3.070200       0.049249         90       [14]       09       [14]       44956.27900       08.049572       3.070200       0.049249         90       [14]       09       [14]       496228       3.322400       0.161700         90       [14]       M02+1161       23488.743000       61.774949       3.021200       0.049249         90       [14]       Mar       [18]       92535.428300       209.785247       3.096500       0.118960         90       [14]       Na+       [18]       129535.428300       209.785247       3.096600       0.189765         90       [14]       Na+       [18]       136919.347000       258.405233       3.193000       0.121921         H       HX       Na+       [18]       136919.347000       258.405233       3.193000       0.21921         H, HS       [2]       Na+       [18]       14995.56700       22.840563	OH [9]	90 [14]	413303.707000	552.209132	3.382200	0.184450	
HC [11] 90 [14] 47758.712600 98.108971 3.148200 0.050385 H4 [12] 90 [14] 34546.22900 90.091910 -3.120200 -0.049249 90 [14] 90 [14] 90 [14] 292504.827000 434.962208 3.322400 0.161700 90 [14] H5 [15] 28368.023500 74.755793 3.020200 0.049249 90 [14] Mg2+ [16] 23488.714900 61.77494 3.021200 0.0409249 90 [14] Mg2+ [16] 23488.714900 61.77494 3.021200 0.0409249 90 [14] Mg2+ [16] 23488.714900 61.77494 3.021200 0.0409249 90 [14] Mg2+ [16] 23488.714900 0.075862 90 [14] Mg2+ [16] 23485.748300 299.785247 3.0905900 0.118900 90 [14] Mg2+ [16] 414996.4955000 510.142000 0.000000 0.000000 0.000000 90 [14] Mg2+ [18] 125.82660 510.142000 0.000000 0.000000 0.000000 90 [14] Mg2+ [18] 125.82660 510.142000 0.000000 0.000000 0.000000 90 [14] Mg2+ [18] 125.826601 4.318247 1.965900 0.121921 N,N2,N3,NA,NE [1] Na+ [18] 136919.347000 258.405233 3.193000 0.121921 H,H5 [2] Na+ [18] 1905.867000 242.24266 3.277000 0.037651 H7 [4] Na+ [18] 1901.324490 16.786482 2.469000 0.037651 H1 [5] Na+ [18] 1909.267000 242.24266 3.277000 0.067765 H7 [4] Na+ [18] 1901.324490 16.786482 2.469000 0.037651 H1 [5] Na+ [18] 1901.324490 16.786482 2.469000 0.37651 H1 [5] Na+ [18] 1901.324490 24.737832 3.309000 0.147551 C,C*,CA,CB,CC,CN,CO,CR,CV,CW [7] Na+ [18] 19290.267000 241.4776590 3.277000 0.066717 0 [8] Na+ [18] 102772.745000 236.132213 3.039000 0.147551 H1 [1] Na+ [18] 190772.745000 236.132213 3.039000 0.147651 H1 [2] Na+ [18] 102772.745000 236.132213 3.039000 0.35567 0 H [9] Na+ [18] 102772.745000 236.132324 3.039000 0.35567 0 H [9] Na+ [18] 102772.745000 236.132324 3.039000 0.37561 H1 [12] Na+ [18] 10278.542330 297.955770 3.137300	HO [10]	90 [14]	0.00000	0.00000	0.000000	0.00000	
H4       112       90       141       34546.229000       82.495572       3.070200       0.049249         90       114       90       114       192504.827000       434.962208       3.322400       0.161700         90       114       Mg2+       115       28368.023500       74.755793       3.020200       0.049249         90       114       Mg2+       116       23488.714900       61.774949       3.021200       0.040617         90       114       CL-       117       2122775.910000       802.591625       4.174200       0.075862         90       114       CL-       117       2122775.910000       6.000000       0.000000       0.000000         90       114       CL-       117       2122775.910000       0.000000       0.000000       0.000000       0.000000         90       114       HW       20       0.000000	HC [11]	90 [14]	47758.712600	98.108971	3.148200	0.050385	
MA [13]       90 [14]       41036.272900       90.901010       3.12000       0.040249         90 [14]       90 [14]       915 [15]       28368.023500       74.755793       3.021200       0.040249         90 [14]       Mg2.1161       2122775.910800       802.591655       4.174200       0.040617         90 [14]       C1- [17]       2122775.910800       802.591655       4.174200       0.078562         90 [14]       OH       1181       92535.428300       209.785247       3.096090       0.118000         90 [14]       OH       119       414390.43900       516.142600       5.16.142600       5.16.775         90 [14]       OH       119       414390.439000       209.785247       3.096090       0.100000         90 [14]       OH       119       414390.439000       258.405233       3.193000       0.121921         NATON Type 1       Atom Type 2       A coefficient       B coefficient       R 1, J       69000       0.037051         18 20, 2, 2, 3, NA, NB [1]       Na+ [18]       136919.347000       228.405233       3.193000       0.21921         19, 14, 19, 12, 12, 14, 136       Na+ [18]       136291.347000       258.405233       3.193000       0.21921         19, 14, 19, 14,	H4 [12]	90 [14]	34546.229000	82.495572	3.070200	0.049249	
90         [14]         90         [14]         H2         292504.827000         434.962208         3.322400         0.161700           90         [14]         Mg2+1[16]         23488.714900         61.774949         3.021200         0.049249           90         [14]         Cl-1171         2122775.910000         802.591625         4.174200         0.049249           90         [14]         Na+ [18]         92355.428300         200.785247         3.096900         0.118900           90         [14]         OW [13]         414990.465600         310.412000         3.4257000         0.100000           90         [14]         OW [13]         414990.465600         310.412000         0.00000         0.000000           90         [14]         OW [13]         414990.465600         310.412000         0.00000         0.00000           90         [14]         HW [20]         0.000000         0.00000         0.00000         0.00000           90         [14]         Nat         [18]         136919.347000         258.405233         3.193000         0.121921           H         HS12         Nat         [18]         136919.347000         258.405233         3.193000         0.121921	HA [13]	90 [14]	41936.272900	90.891910	3.120200	0.049249	
90       14]       H5       15       28368.023500       74.755793       3.020200       0.049249         90       141       C1- [17]       2122775.910000       802.591625       4.174200       0.075862         90       141       C1- [17]       2122775.910000       802.591625       4.174200       0.075862         90       141       NH       181       92535.428300       209.785247       3.095000       0.190000         90       141       NH       120       0.000000       0.000000       0.000000       0.000000         90       141       HW       [20]       0.000000       0.000000       0.000000       0.000000         90       141       HW       [20]       0.000000       0.000000       0.000000       0.000000         90       141       HW       [20]       0.000000       258.405233       3.193000       0.121921         N,N2,N3,NA,NB       [1]       Na+ [18]       136919.347000       258.405233       3.193000       0.121921         H,HS       [2]       Na+ [18]       136919.347000       258.405233       3.193000       0.121921         L,HS       [2]       Na+ [18]       136919.347000       263.405061       3	90 [14]	90 [14]	292504.827000	434.962208	3.322400	0.161700	
90 [14] M2+ [16] 23488.714900 61.774949 3.021200 0.040617 90 [14] Cl- [17] 212775.910000 802.5916.25 4.174200 0.075862 90 [14] Na+ [18] 92535.428300 209.785247 3.096900 0.118900 90 [14] WH [20] 0.000000 0.000000 0.000000 0.000000 0.000000	90 [14]	H5 [15]	28368.023500	74.755793	3.020200	0.049249	
90 [14] C.L. [17] 2122775.910000 802.591625 4.174200 0.075862 90 [14] Na+ [18] 92535.428300 209.785247 3.90600 0.118900 90 [14] HW [20] 0.000000 0.000000 0.000000 0.000000 90 [14] HW [20] 0.000000 0.000000 0.000000 0.000000 N,N2,N3,NA,NB [1] Na+ [18] 136919.347000 258.405233 3.193000 0.121921 H,HS [2] Na+ [18] 125.820601 4.318247 1.999000 0.037051 2C,3C,CB,CT,CX [3] Na+ [18] 19995.867000 242.242668 3.277000 0.097805 HP [4] Na+ [18] 1901.324490 16.786482 2.469000 0.037051 HH [5] Na+ [18] 1146.52960 32.471955 2.755000 0.037051 S,SH [6] Na+ [18] 316107.989000 432.373832 3.369000 0.147851 C,C*,CA,CB,CC,CN,CO,CR,CV,CW [7] Na+ [18] 132990.267000 214.778698 3.277000 0.086717 0 [8] Na+ [18] 102772.745000 230.133213 3.090000 0.135507 0 H [9] Na+ [18] 102772.745000 230.133213 3.090000 0.135507 0 H [10] Na+ [18] 10911.930700 40.214472 2.856000 0.037051 H4 [12] Na+ [18] 10911.930700 40.214472 2.856000 0.037051 H4 [12] Na+ [18] 10911.930700 40.214472 2.856000 0.037051 H4 [12] Na+ [18] 10911.930700 40.214472 2.78000 0.037051 H4 [12] Na+ [18] 00000 0.000000 0.000000 0.000000 HC [11] Na+ [18] 10911.930700 40.214472 2.78000 0.037051 H4 [12] Na+ [18] 000000 0.000000 0.000000 0.0000000 H6 [10] Na+ [18] 000000 0.000000 0.000000 0.0000000 H6 [10] Na+ [18] 000000 0.000000 0.000000 0.0000000 0.000000	90 [14]	Mg2+ [16]	23488.714900	61.774949	3.021200	0.040617	
90         [14]         Na+         [18]         92535.428300         209.785247         3.096900         0.118900           90         [14]         0W         [19]         414996.465600         510.142060         3.429500         0.000000           90         [14]         HW         [20]         0.000000         0.000000         0.000000         0.000000           > printLJMatrix :Na+         Atom Type 1         Atom Type 2         A coefficient         B coefficient         R i, j         Eps i, j           N,N2,N3,NA,NB         [1]         Na+         [18]         12520601         4.31827         1.969000         0.097805           2C, 3C, C8, CT, CX         [3]         Na+         [18]         149995.867000         228.405233         3.193000         0.121921           H         H5         Na+         [18]         149995.867000         248.471         1.969000         0.097805           2C, 3C, C8, CT, CX         [3]         Na+         [18]         14995.867000         24.471855         2.756000         0.097805           H1         [5]         Na+         [18]         7114.652960         32.471955         2.756000         0.037651           C, C*, CA, CB, CC, CN, CO, CR, CV, CW         I71	90 [14]	<u>Cl-[17]</u>	2122775.910000	802.591625	4.174200	0.075862	
90         [14]         0W         [19]         414936.465000         510.142660         3.429500         0.150775         -           90         [14]         HW         [20]         0.000000         0.00000         0.00000         0.00000         0.000000         0.000000         0.000000         0.00000         0.00000         0.00000         0.00000         0.00000         0.00000         0.00000         0.00000         0.00000         0.00000         0.00000         0.00000         0.00000         0.00000         0.00000         0.000000         0.000000         0.00000<	90 [14]	Na+ [18]	92535.428300	209.785247	3.096900	0.118900	
90 [14]       HW [20]       0.000000       0.000000       0.000000         > printLJMatrix :Na+         Atom Type 1       Atom Type 2       A coefficient       B coefficient       R 1,j       Eps 1,j         N,N2,N3,NA,NB [1]       Na+ [18]       136919.347000       258.405233       3.193000       0.121921         H,HS [2]       Na+ [18]       125.820601       4.318247       1.969000       0.037051         2C,3C,C8,CT,CX [3]       Na+ [18]       149995.867000       242.242668       3.277000       0.097805         H1 [5]       Na+ [18]       7114.652960       32.471955       2.756000       0.037051         H1 [5]       Na+ [18]       7114.652960       32.471955       2.756000       0.037051         H1 [5]       Na+ [18]       1316107.989000       432.373822       3.369000       0.147851         C,C*,CA,CB,CC,CN,CO,CR,CV,CW [7]       Na+ [18]       13211.682800       209.807371       3.030200       0.135563         0H [9]       Na+ [18]       102772.745000       236.132213       3.990600       0.37051         H4 [12]       Na+ [18]       10911.930700       40.214472       2.856000       0.037051         H4 [12]       Na+ [18]       0.000000       0.0362216       2.	90 [14]	OW [19]	414998.465000	510.142660	3.429500	0.156775	
<pre>&gt; printLJMatrix :Na+</pre>	90 [14]	HW [20]	0.00000	0.00000	0.000000	0.000000	
Atom Type 1         Atom Type 2         A coefficient         B coefficient         R i,j         Eps i,j           N,N2,N3,NA,NB [1]         Na+ [18]         136919.347000         258.405233         3.193000         0.121921           H,HS [2]         Na+ [18]         125.820601         4.318247         1.969000         0.037051           2C,3C,C8,CT,CX [3]         Na+ [18]         149995.867000         242.242668         3.277000         0.097805           HP [4]         Na+ [18]         1901.324490         16.786482         2.469000         0.037051           HJ [5]         Na+ [18]         1901.324490         16.786482         2.469000         0.037051           S,SH [6]         Na+ [18]         16107.989000         432.373832         3.59000         0.147851           C,C*,CA,CB,CC,CN,CO,CR,CV,CW [7]         Na+ [18]         132990.267000         214.778698         3.277000         0.086717           0         [8]         Na+ [18]         102772.745000         236.133213         3.090000         0.1355367           0H [9]         Na+ [18]         10911.937070         40.21472         2.856000         0.037051           H4 [12]         Na+ [18]         7650.430290         33.290660         2.778000         0.036216      <	> printLJMatrix :Na+						
Atom type 1       Atom type 2       Atom type 2       Atom type 2       Atom type 2       Atom type 1       R 1, j       Lps 1, j         N,N2,N3,NA,NB [1]       Na+ [18]       136919.347000       258.405233       3.193000       0.121921         H,HS [2]       Na+ [18]       125.820601       4.318247       1.969000       0.037051         2C,3C,C8,CT,CX [3]       Na+ [18]       1991.324490       16.786482       2.469000       0.037051         HI [4]       Na+ [18]       7114.652960       32.471955       2.756000       0.037051         H1 [5]       Na+ [18]       316107.989000       432.373832       3.369000       0.147851         C,C*,CA,CB,CC,CN,CO,CR,CV,CW [7]       Na+ [18]       112990.267000       214.778698       3.277000       0.0866717         0 [8]       Na+ [18]       1211.682800       209.807371       3.030200       0.135507         0H [9]       Na+ [18]       0.000000       0.000000       0.000000       0.000000       0.000000         H4 [12]       Na+ [18]       10911.930700       40.214472       2.856000       0.37051         H4 [12]       Na+ [18]       0911.930700       40.214472       2.856000       0.037051         H4 [12]       Na+ [18]       092535.428			A coefficient		Dii	Enc i i	
N, N2, N3, NA, NB [1]       Na+ [18]       136919.347000       258.405233       3.193000       0.121921         H, HS [2]       Na+ [18]       125.820601       4.318247       1.969000       0.037851         2C, 3C, C8, CT, CX [3]       Na+ [18]       149995.867000       242.242668       3.277000       0.037051         H1       [5]       Na+ [18]       1901.324490       16.786482       2.469000       0.037051         H1       [5]       Na+ [18]       316107.989000       432.373832       3.369000       0.147851         C, C*, CA, CB, CC, CN, CO, CR, CV, CW [7]       Na+ [18]       131210.682800       209.807371       3.036200       0.135507         O [8]       Na+ [18]       102172.745000       236.133213       3.090000       0.000000         O [8]       Na+ [18]       10911.930700       40.214472       2.856000       0.037051         H4       [12]       Na+ [18]       10911.930700       40.214472       2.856000       0.030051         H4       [12]       Na+ [18]       10911.930700       40.214472       2.856000       0.037051         H4       [12]       Na+ [18]       0475.584230       37.51866       2.778000       0.036216         H5       Na+ [18] <t< td=""><td>Асот туре т</td><td>Alom Type 2</td><td>A coefficient</td><td>B coefficient</td><td>К 1, ј</td><td>Eps I,J</td></t<>	Асот туре т	Alom Type 2	A coefficient	B coefficient	К 1, ј	Eps I,J	
H,HS [2]       Na+ [18]       125.820601       4.318247       1.969000       0.037051         2C,3C,C8,CT,CX [3]       Na+ [18]       149995.867000       242.242668       3.277000       0.097805         HP [4]       Na+ [18]       1901.324490       16.786482       2.46000       0.037051         H1 [5]       Na+ [18]       1901.324490       16.786482       2.45000       0.037051         S,SH [6]       Na+ [18]       316107.989000       432.373832       3.369000       0.147851         C,C*,CA,CB,CC,CN,CO,CR,CV,CW [7]       Na+ [18]       132990.267000       214.778698       3.277000       0.086717         0 [8]       Na+ [18]       102772.745000       236.133213       3.090000       0.135536         0H [9]       Na+ [18]       102772.745000       236.133213       3.090000       0.135636         H0 [10]       Na+ [18]       10911.930700       40.214472       2.856000       0.036216         H4       [12]       Na+ [18]       0476       584230       37.951466       2.828000       0.036216         H4       [13]       Na+ [18]       0476       584230       37.951466       2.828000       0.036216         H5       [15]       Na+ [18]       0476       5	N,N2,N3,NA,NB [1]	Na+ [18]	136919.347000	258.405233	3.193000	0.121921	
2C, 3C, C8, CT, CX       [3]       Na+       [18]       149995.867000       242.242668       3.277000       0.097805         HP       [4]       Na+       [18]       1901.324490       16.786482       2.469000       0.037051         H1       [5]       Na+       [18]       7114.652960       32.471955       2.756000       0.037051         S, SH       [6]       Na+       [18]       316107.989000       432.373832       3.369000       0.147851         C, C*, CA, CB, CC, CN, CO, CR, CV, CW       [7]       Na+       [18]       132990.267000       214.778698       3.277000       0.0866717         0       [8]       Na+       [18]       102772.745000       236.13213       3.090000       0.135507         0H       [9]       Na+       [18]       102772.745000       236.13213       3.090000       0.135636         H0       [10]       Na+       [18]       10911.930700       40.214472       2.856000       0.037051         H4       [12]       Na+       [18]       0476.584230       37.951466       2.828000       0.036216         H4       [13]       Na+       [18]       0476.584230       37.951466       2.828000       0.036216	H,HS [2]	Na+ [18]	125.820601	4.318247	1.969000	0.037051	
HP       [4]       Na+       [18]       1901.324490       16.786482       2.469000       0.037051         H1       [5]       Na+       [18]       7114.652960       32.471955       2.756000       0.037051         S,SH       [6]       Na+       [18]       316107.989000       432.373832       3.369000       0.147851         C,C*,CA,CB,CC,CN,CO,CR,CV,CW       [7]       Na+       [18]       31211.682800       209.807371       3.030200       0.135507         O       [8]       Na+       [18]       102772.745000       236.133213       3.090000       0.135636         HO       [10]       Na+       [18]       0.000000       0.000000       0.000000       0.000000         H4       [12]       Na+       [18]       10911.930700       40.214472       2.856000       0.037051         H4       [12]       Na+       [18]       0476.584230       37.951466       2.828000       0.036216         H4       [12]       Na+       [18]       0476.584230       37.951466       2.828000       0.036216         H4       [12]       Na+       [18]       0476.584230       37.951466       2.828000       0.036216         H4       [12]	2C.3C,C8,CT,CX [3]	Na+ [18]	149995.867000	242,242668	3.277000	0.097805	
H1       [5]       Na+       [18]       7114.652960       32.471955       2.756000       0.037051         S,SH       [6]       Na+       [18]       316107.989000       432.373832       3.369000       0.147851         C,C*,CA,CB,CC,CN,CO,CR,CV,CW       [7]       Na+       [18]       132990.267000       214.778698       3.277000       0.086717         O       [8]       Na+       [18]       81211.682800       209.807371       3.030200       0.135507         OH       [9]       Na+       [18]       102772.745000       236.133213       3.09000       0.135636         H0       [10]       Na+       [18]       0.000000       0.000000       0.000000       0.000000         H4       [12]       Na+       [18]       10911.930700       40.214472       2.856000       0.037051         H4       [12]       Na+       [18]       0476.584230       37.951466       2.828000       0.036216         HA       [13]       Na+       [18]       9476.584230       2.728000       0.036216         H4       [12]       Na+       [18]       052.212920       29.853493       2.728000       0.036216         Mg2+       [16]       Na+	HP [4]	Na+ [18]	1901.324490	16.786482	2.469000	0.037051	
S,SH [6]       Na+ [18]       316107.989000       432.373832       3.369000       0.147851         C,C*,CA,CB,CC,CN,CO,CR,CV,CW [7]       Na+ [18]       132990.267000       214.778698       3.277000       0.086717         O [8]       Na+ [18]       81211.682800       209.807371       3.030200       0.135507         OH [9]       Na+ [18]       102772.745000       236.133213       3.090000       0.136366         HO [10]       Na+ [18]       100000       0.000000       0.000000       0.000000         HC [11]       Na+ [18]       10911.930700       40.214472       2.856000       0.37051         H4 [12]       Na+ [18]       7650.430290       33.290660       2.778000       0.036216         90       [14]       Na+ [18]       92535.428300       209.785247       3.096900       0.118900         H5 [15]       Na+ [18]       9152.212920       29.853493       2.728000       0.036216         Mg2+ [16]       Na+ [18]       5096.198070       24.674882       2.729000       0.029868         C1- [17]       Na+ [18]       653416.059000       381.844565       3.882000       0.055786         Na+ [18]       Na+ [18]       1552.0581800       73.677916       2.738000       0.087439	H1 [5]	Na+ [18]	7114.652960	32.471955	2.756000	0.037051	
C,C*,CA,CB,CC,CN,CO,CR,CV,CW [7] Na+ [18] 132990.267000 214.778698 3.277000 0.086717 0 [8] Na+ [18] 81211.682800 209.807371 3.030200 0.135507 OH [9] Na+ [18] 102772.745000 236.133213 3.090000 0.135636 HO [10] Na+ [18] 0.000000 0.000000 0.000000 0.000000 HC [11] Na+ [18] 10911.930700 40.214472 2.856000 0.037051 H4 [12] Na+ [18] 7650.430290 33.290660 2.778000 0.036216 HA [13] Na+ [18] 92535.428300 209.785247 3.096900 0.118900 H5 [15] Na+ [18] 92535.428300 209.785247 3.096900 0.118900 H5 [15] Na+ [18] 6152.212920 29.853493 2.728000 0.036216 Mg2+ [16] Na+ [18] 5096.198070 24.674882 2.729000 0.029868 C1- [17] Na+ [18] 653416.059000 381.844565 3.882000 0.055786 Na+ [18] Na+ [18] 1550.581800 73.677916 2.738000 0.087439 Na+ [18] 0W [19] 104820.861000 219.857570 3.137300 0.115286 Na+ [18] HW [20] 0.000000 0.000000 0.000000 0.000000	S,SH [6]	Na+ [18]	316107.989000	432.373832	3.369000	0.147851	
Na+       18]       Na+       18]       81211.682800       209.807371       3.030200       0.135507         0H       [9]       Na+       18]       102772.745000       236.133213       3.090000       0.135636         H0       [10]       Na+       [18]       0.000000       0.000000       0.000000       0.000000         HC       [11]       Na+       [18]       10911.930700       40.214472       2.856000       0.037051         H4       [12]       Na+       [18]       10911.930700       40.214472       2.856000       0.036216         H4       [13]       Na+       [18]       9476       584230       37.951466       2.828000       0.036216         H4       [13]       Na+       [18]       92535.428300       209.785247       3.096900       0.118900         H5       [15]       Na+       [18]       6152.212920       29.853493       2.728000       0.029868         C1-       [17]       Na+       [18]       5096.198070       24.674882       2.729000       0.029868         C1-       [17]       Na+       [18]       552.0581800       73.677916       2.738000       0.057786         Na+       [18]       <	C,C*,CA,CB,CC,CN,CO,CR,CV,CW [7]	Na+ [18]	132990.267000	214.778698	3.277000	0.086717	
0H       [9]       Na+       18]       102772.745000       236.133213       3.090000       0.135636         H0       [10]       Na+       [18]       0.000000       0.000000       0.000000       0.000000         HC       [11]       Na+       [18]       10911.930700       40.214472       2.856000       0.037051         H4       [12]       Na+       [18]       7650.430290       33.290660       2.778000       0.036216         H4       [13]       Na+       [18]       9476       584230       37<451466	0 [8]	Na+ [18]	81211.682800	209.807371	3.030200	0.135507	
H0 [10]       Na+ [18]       0.000000       0.000000       0.000000         HC [11]       Na+ [18]       10911.930700       40.214472       2.856000       0.037051         H4 [12]       Na+ [18]       7650.430290       33.290660       2.778000       0.036216         HA [13]       Na+ [18]       9476       584230       37.051466       2.828000       0.036216         90 [14]       Na+ [18]       92535.428300       209.785247       3.096900       0.118900         H5 [15]       Na+ [18]       0152.212920       29.853493       2.728000       0.036216         Mg2+ [16]       Na+ [18]       5096.198070       24.674882       2.729000       0.029868         C1- [17]       Na+ [18]       653416.059000       381.844565       3.882000       0.055786         Na+ [18]       Na+ [18]       15520.581800       73.677916       2.738000       0.087439         Na+ [18]       OW [19]       104820.861000       219.857570       3.137300       0.115286         Na+ [18]       HW [20]       0.000000       0.000000       0.000000       0.000000	OH [9]	Na+ [18]	102772.745000	236.133213	3.090000	0.135636	
HC       [11]       Na+       [18]       10911.930700       40.214472       2.856000       0.037051         H4       [12]       Na+       [18]       7650.430290       33.290660       2.778000       0.036216         HA       [13]       Na+       [18]       9676.584230       37.951466       2.828000       0.036216         90       [14]       Na+       [18]       92535.428300       209.785247       3.096900       0.118900         H5       [15]       Na+       [18]       6152.212920       29.853493       2.728000       0.036216         Mg2+       [16]       Na+       [18]       5096.198070       24.674882       2.729000       0.029868         C1-       [17]       Na+       [18]       653416.059000       381.844565       3.882000       0.055786         Na+       [18]       Na+       [18]       15520.581800       73.677916       2.738000       0.087439         Na+       [18]       0W       [19]       104820.861000       219.857570       3.137300       0.152286         Na+       [18]       HW       [20]       0.000000       0.000000       0.000000	HO [10]	Na+ [18]	0.00000	0.000000	0.000000	0.000000	
H4       [12]       Na+       [18]       7650.430290       33.290660       2.778000       0.036216         HA       [13]       Na+       [18]       9476       584230       37       051466       2       828000       0       036216         90       [14]       Na+       [18]       92535.428300       209.785247       3.096900       0.118900         H5       [15]       Na+       [18]       6152.212920       29.853493       2.728000       0.036216         Mg2+       [16]       Na+       [18]       5096.198070       24.674882       2.729000       0.029868         Cl-       [17]       Na+       [18]       653416.059000       381.844565       3.882000       0.055786         Na+       [18]       Na+       [18]       15520.581800       73.677916       2.738000       0.087439         Na+       [18]       OW       [19]       104820.861000       219.857570       3.137300       0.115286         Na+       [18]       HW       [20]       0.000000       0.000000       0.000000	HC [11]	Na+ [18]	10911.930700	40.214472	2.856000	0.037051	
HA       13       Na+       18       9476       584230       37       951466       2       828000       0       936216         90       [14]       Na+       [18]       92535.428300       209.785247       3.096900       0.118900         H5       [15]       Na+       [18]       6152.212920       29.853493       2.728000       0.036216         Mg2+       [16]       Na+       [18]       5096.198070       24.674882       2.729000       0.029868         Cl-       [17]       Na+       [18]       653416.059000       381.844565       3.882000       0.055786         Na+       [18]       Na+       [18]       15520.581800       73.677916       2.738000       0.087439         Na+       [18]       OW       [19]       104820.861000       219.857570       3.137300       0.115286         Na+       [18]       HW       [20]       0.000000       0.000000       0.000000	H4 [12]	Na+ [18]	7650.430290	33.290660	2.778000	0.036216	
90         [14]         Na+         [18]         92535.428300         209.785247         3.096900         0.118900           H5         [15]         Na+         [18]         6152.212920         29.853493         2.728000         0.036216           Mg2+         [16]         Na+         [18]         5096.198070         24.674882         2.729000         0.029868           C1-         [17]         Na+         [18]         653416.059000         381.844565         3.882000         0.055786           Na+         [18]         15520.581800         73.677916         2.738000         0.087439           Na+         [18]         0W         [19]         104820.861000         219.857570         3.137300         0.115286           Na+         [18]         HW         [20]         0.000000         0.000000         0.000000	HA [13]	Na+ [18]	9476 584230	37 051466	2 828000	0 036216	
H5 [15]       Na+ [18]       6152.212920       29.853493       2.728000       0.036216         Mg2+ [16]       Na+ [18]       5096.198070       24.674882       2.729000       0.029868         Cl- [17]       Na+ [18]       653416.059000       381.844565       3.882000       0.055786         Na+ [18]       Na+ [18]       15520.581800       73.677916       2.738000       0.087439         Na+ [18]       0W [19]       104820.861000       219.857570       3.137300       0.115286         Na+ [18]       HW [20]       0.000000       0.000000       0.000000	90 [14]	Na+ [18]	92535.428300	209.785247	3.096900	0.118900	
Mg2+[16]Na+[18]5096.19807024.6748822.7290000.029868Cl-[17]Na+[18]653416.059000381.8445653.8820000.055786Na+[18]Na+[18]15520.58180073.6779162.7380000.087439Na+[18]0W[19]104820.861000219.8575703.1373000.115286Na+[18]HW[20]0.0000000.0000000.000000	H5 [15]	Na+ [18]	6152.212920	29.853493	2./28000	0.036216	
Cl-[17]Na+[18]653416.059000381.8445653.8820000.055786Na+[18]Na+[18]15520.58180073.6779162.7380000.087439Na+[18]OW[19]104820.861000219.8575703.1373000.115286Na+[18]HW[20]0.0000000.00000000.000000	Mg2+ [16]	Na+ [18]	5096.198070	24.674882	2.729000	0.029868	
Na+[18]Na+[18]15520.58180073.6779162.7380000.087439Na+[18]OW[19]104820.861000219.8575703.1373000.115286Na+[18]HW[20]0.0000000.00000000.0000000	Čl- [17]	Na+ [18]	653416.059000	381.844565	3.882000	0.055786	
Na+ [18] 0W [19] 104820.861000 219.857570 3.137300 0.115286 Na+ [18] HW [20] 0.000000 0.000000 0.000000 0.000000	Na+ [18]	Na+ [18]	15520.581800	73.677916	2.738000	0.087439	
Na+ [18] HW [20] 0.000000 0.000000 0.000000 0.000000	Na+ [18]	OW [19]	104820.861000	219.857570	3.137300	0.115286	
	Na+ [18]	HW [20]	0.00000	0.00000	0.000000	0.000000	

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## Well done; you're good to go!