



Building LAMMPS data files with car/mdf files and the msi2Imp utility

Jeffery A. Greathouse

Sandia National Laboratories, Albuquerque, New Mexico

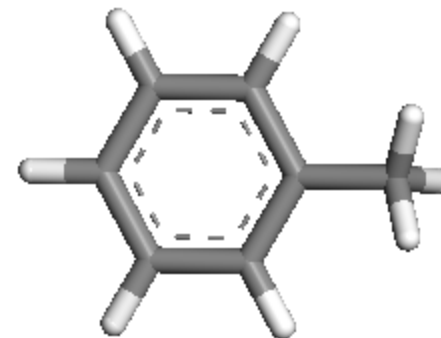
Outline

- ▶ Description of files
 - LAMMPS data file
 - Structure files (car/mdf)
 - Force field files (frc)
 - msi2Imp.exe
- } Biosym/Discover software
-
- ▶ Mineral with limited bonding (kaolinite)
 - ▶ Bonded organic molecule (toluene)

LAMMPS Data Files

- ▶ http://lammps.sandia.gov/doc/read_data.html
- ▶ Typical components (**toluene.lammps05**)
 - Summary of molecular connectivity
 - Cell dimensions
 - Force field parameters (pair, bond, angle, dihedral, improper)
 - Atom info (molecule #, atom type #, charge, xyz coordinates)
 - Bond info (bonds, angles, etc)
- ▶ Examples in LAMMPS distribution

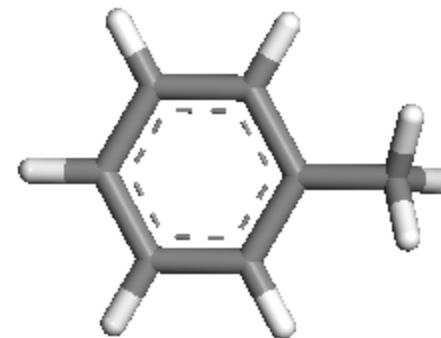
Structure Files



► car file (coordinates, atom type, charge)

C1	-0.692663292	-0.094096410	0.003399037	XXXX 1	cp	C	-0.100
C2	0.080988729	-1.425449986	0.004347065	XXXX 1	cp	C	-0.100
C3	1.620876319	-1.420834453	0.005671437	XXXX 1	cp	C	-0.100
C4	2.386905208	-0.085003697	-0.002079692	XXXX 1	cp	C	-0.100
C5	1.613536848	1.246298529	-0.026904058	XXXX 1	cp	C	0.000
C6	0.073572216	1.241704742	-0.004902500	XXXX 1	cp	C	-0.100
C7	2.379381006	2.581705596	0.007764760	XXXX 1	c3	C	-0.300
H1	-1.832488967	-0.097446130	0.009999447	XXXX 1	h	H	0.100
H2	-0.486334530	-2.414248925	0.007052748	XXXX 1	h	H	0.100
H3	2.193596249	-2.406396682	0.013631449	XXXX 1	h	H	0.100
H4	3.526773693	-0.081542221	0.008067005	XXXX 1	h	H	0.100
H5	-0.499289128	2.227113274	0.002830637	XXXX 1	h	H	0.100
H6	2.624394086	2.906106279	-1.057242639	XXXX 1	h	H	0.100
H7	3.346362304	2.450326318	0.597088580	XXXX 1	h	H	0.100
H8	1.733495243	3.376908124	0.507943882	XXXX 1	h	H	0.100

Structure Files



► mdf file (atom type, charge, bonding information)

XXXX_1:C1	C	cp	?	0	0	-0.1000	0	0	8	1.0000	0.0000	C2/1.5	C6/1.5	H1
XXXX_1:C2	C	cp	?	0	0	-0.1000	0	0	8	1.0000	0.0000	C3/1.5	C1/1.5	H2
XXXX_1:C3	C	cp	?	0	0	-0.1000	0	0	8	1.0000	0.0000	C2/1.5	C4/1.5	H3
XXXX_1:C4	C	cp	?	0	0	-0.1000	0	0	8	1.0000	0.0000	C3/1.5	C5/1.5	H4
XXXX_1:C5	C	cp	?	0	0	0.0000	0	0	8	1.0000	0.0000	C4/1.5	C6/1.5	C7
XXXX_1:C6	C	cp	?	0	0	-0.1000	0	0	8	1.0000	0.0000	C5/1.5	C1/1.5	H5
XXXX_1:C7	C	c3	?	0	0	-0.3000	0	0	8	1.0000	0.0000	C5	H6	H7
XXXX_1:H1	H	h	?	0	0	0.1000	0	0	8	1.0000	0.0000	C1		
XXXX_1:H2	H	h	?	0	0	0.1000	0	0	8	1.0000	0.0000	C2		
XXXX_1:H3	H	h	?	0	0	0.1000	0	0	8	1.0000	0.0000	C3		
XXXX_1:H4	H	h	?	0	0	0.1000	0	0	8	1.0000	0.0000	C4		
XXXX_1:H5	H	h	?	0	0	0.1000	0	0	8	1.0000	0.0000	C6		
XXXX_1:H6	H	h	?	0	0	0.1000	0	0	8	1.0000	0.0000	C7		
XXXX_1:H7	H	h	?	0	0	0.1000	0	0	8	1.0000	0.0000	C7		
XXXX_1:H8	H	h	?	0	0	0.1000	0	0	8	1.0000	0.0000	C7		

Force Field Files

- ▶ These files are in the Biosym/Discover format and available in the LAMMPS distribution (.../tools/msi2Imp)
 - cff91.frc
 - **cvff.frc**
 - cvff_aug.frc
 - pcff.frc (pcff.rlb and pcff_templates.dat also needed)
- ▶ Information contained in frc files
 - Atom types
 - Energy expressions and parameters
 - Atomic charge assignments (**not used by msi2Imp**)
- ▶ Build you own frc file (**clayff.frc**)

msi2Imp.exe

- ▶ Available in LAMMPS distribution (.../tools/msi2Imp)
- ▶ Written in C
- ▶ Updated as of LAMMPS 2005
- ▶ Reads molecular information from structure files and produces a LAMMPS data file
- ▶ Syntax:

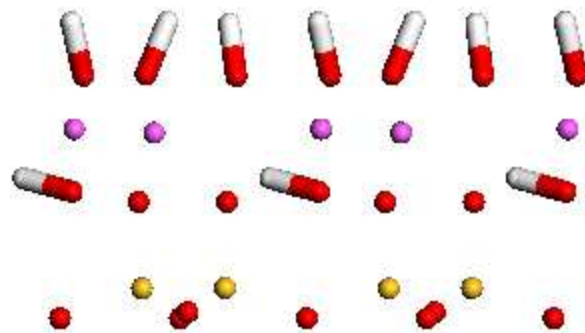
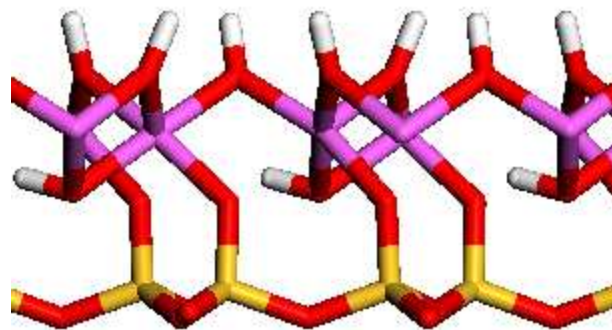
msi2Imp.exe *root* -frc *frc_file*

root = root name of car/mdf files (toluene.car, toluene.mdf)

frc_file = Biosym/Discover force field file

Example – kaolinite $\text{Al}_2\text{Si}_2\text{O}_5(\text{OH})_4$

- ▶ Fully bonded model
 - Created with Materials Studio software
 - Atom types assigned manually
- ▶ Nonbonded model for LAMMPS simulations (except for hydroxyl groups)
- ▶ Build kaolinite data file from **kaolinite.car** and **kaolinite.mdf**



Example – toluene vapor

- ▶ Atom types and charges assigned automatically with Materials Studio software
- ▶ All other parameters assigned automatically from `cvff.frc`
 - pair coeffs
 - bond coeffs
 - angle coeffs
 - dihedral coeffs
 - improper coeffs
- ▶ Build toluene data file from `toluene.car` and `toluene.mdf`

