GROMACS - Bug #957
Spurious parameters for Argon in OPLS-AA and Charmm27
06/15/2012 01:18 AM - Lutz Maibaum

| Status:    | Closed      |
| Priority:  | Normal      |
| Assignee:  |             |
| Category:  |             |
| Target version: |            |
| Affected version - extra info: | 4.5.5       |
| Affected version: |             |

| Difficulty: | uncategorized |

Description
The parameter file ffnonbonded.itp for the OPLS-AA force field defines two different non-bonded interactions for Argon atoms:

```
opls_097   Ar  18   39.94800     0.000       A    3.40100e-01  9.78638e-01 ; SIG
```

and

```
Ar         Ar     18    39.94800     0.000       A    3.41000e-01  2.74580e-02
```

The first one seems reasonable, but the second one has a Lennard-Jones epsilon that seems way too small (by a factor of about 35). The Charmm27 force field contains only the spurious second definition for the argon parameters.

It's not clear to me where this value for epsilon comes form, but it doesn't look right to me. Reasonable values for the energy parameter can be found here:


It would be great if someone could look into this, and either correct the parameter or remove the argon definition from these force fields. For reference, it looks like this problem has been spotted before:


Associated revisions

**Revision 6d577e17 - 11/16/2012 11:59 PM - Roland Schulz**

Removing Zn and Ar non-OPLS atom types

Some parameters were clearly wrong and the source of them was not documented. They can be added back in but then the source needs to be documented.

Add source for Fe2+.

Leaving Cu2+, Fe2+ and SI given their source is documented.

Fixes #957

Change-Id: i82a5b7ae4a54ab2aeb5690ceaa9156146a9819250

**Revision 05d7d989 - 05/07/2015 04:17 PM - Berk Hess**

Removed non-ff atomtypes from oplsaa and charm27

Removed atom types Cu2+, Fe2+ and SI from oplsaa and charm27, since they are not part of the official force fields.

Refs #957.

Change-Id: lc8ebdbbee62b4441184a54a580b83849ba21ca978

History

#1 - 10/17/2012 10:20 PM - Roland Schulz
Could you upload your suggested parameters to gerrit.gromacs.org?

#2 - 11/10/2012 08:30 PM - Roland Schulz
- Status changed from New to In Progress

#3 - 12/20/2012 06:14 PM - Erik Lindahl
- Status changed from In Progress to Closed

#4 - 05/07/2015 10:05 AM - Gerrit Code Review Bot
Gerrit received a related patchset '2' for Issue #957.
Uploader: Berk Hess (hess@kth.se)
Change-Id: Ic8ebdbee62b4441184a54a580b83849ba21ca978
Gerrit URL: https://gerrit.gromacs.org/4555

#5 - 01/28/2020 11:57 AM - Irvin Moss
who invented the internet