GROMACS - Bug #2407
Incorrect grompp net charge warning
02/13/2018 12:55 PM - Berk Hess

Status: Closed
Priority: Normal
Assignee: Berk Hess
Category: preprocessing (pdb2gmx, grompp)
Target version: 2018.1
Affected version - extra info: 
Affected version: 2016

Description

grompp only sums the charges over the molecule blocks in the system up to molecule type count and not to the molecule block count. So if the same molecule type appears in multiple, non consecutive, molecule blocks, the total charge sum can be incorrect when there are molecules with net charge.

Associated revisions

Revision 8289af83 - 02/14/2018 09:57 AM - Berk Hess
Fix grompp net charge check
The grompp check for the net charge would ignore molecule blocks at the end when molecule types are used in multiple, non consecutive molecule blocks.
Fixes #2407
Change-id: l4e7c6c609da99025174180f9d4037ac9f9fd7fc

Revision 93ac68d4 - 02/14/2018 09:58 AM - Berk Hess
Fix grompp net charge check
The grompp check for the net charge would ignore molecule blocks at the end when molecule types are used in multiple, non consecutive molecule blocks.
Fixes #2407
Change-id: l4e7c6c609da99025174180f9d4037ac9f9fd7fc

History

#1 - 02/13/2018 12:56 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #2407.
Uploader: Berk Hess (hess@kth.se)
Change-id: gromacs~release-2018~I4e7c6c609da99025174180f9d4037ac9f9fd7fc
Gerrit URL: https://gerrit.gromacs.org/7569

#2 - 02/13/2018 12:57 PM - Berk Hess
- Status changed from In Progress to Fix uploaded

#3 - 02/14/2018 09:58 AM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #2407.
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-id: gromacs~release-2016~I4e7c6c609da99025174180f9d4037ac9f9fd7fc
Gerrit URL: https://gerrit.gromacs.org/7575

#4 - 02/14/2018 10:15 AM - Berk Hess
- Status changed from Fix uploaded to Resolved
Applied in changeset 8289af8355468662d4eb157cc505311260aba11aa.

#5 - 02/14/2018 01:30 PM - Berk Hess
Applied in changeset 93ac68d4a53df45289c9de89aa56b275afab18a.

#6 - 02/16/2018 03:26 PM - Mark Abraham
- Status changed from Resolved to Closed