GROMACS - Bug #359

Missing bond in chloroform .rtp files

10/21/2009 05:47 PM - Justin Lemkul

Status:	Closed		
Priority:	Normal		
Assignee:	Erik Lindahl		
Category:	mdrun		
Target version:	4.0		
Affected version - extra info:		**Difficulty:**	uncategorized
Affected version:			

Description

There is a problem with the CHCL3 directive in all Gromos96 .rtp files. None of them define a bond between C and H. For ffG43a1, ffG43a2, and ffG45a3, the correct line should read:

CChl HChl gb_36

For ffG53a5 and ffG53a6, the correct line should be:

CChl HChl gb_39

As well, the atom names given in the .rtp entry are impossible to satisfy in a .pdb file, given the fact that the chlorine atoms are five characters long. I would suggest they be changed to, i.e., CL1, CL2, and CL3. I have implemented this setup in my own files without issue.

History

#1 - 11/09/2009 05:31 PM - Berk Hess

There is no missing bond here.
All solvent models in GROMOS, including chloroform, are completely rigid.
All bonds should be constrained. Adding the bond, and thus constraint,
you suggest result in an more constraints than DOF's, which should be avoided.

The atom naming is unfortunate, but I don't think we should adapt the atom
names to the most restrictive format.

Berk