GROMACS - Feature #1671

suggestion to check most up-to-date values for constants

01/14/2015 03:24 AM - Chris Neale

<table>
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Description

In gromacs 4.6.7, I find the following definitions in the include directory:

```c
#define BOLTZMANN (1.380658e-23)  /* (J/K) */
#define AVOGADRO (6.0221367e23)  /* () */
```

Neither of these definitions exactly matches the values that one finds from wikipedia. I know that wikipedia is not always correct, but if these constants have been determined at greater precision since the gromacs code was originally written then perhaps they could use another look.

Associated revisions

Revision 1ee3b155 - 06/23/2015 06:26 PM - Erik Lindahl
Updated physical constants from NIST 2010 CODATA

Minor fixes (usually to the 5-6th decimal), and more constants have been derived the basic ones instead of specifying values directly. The units section in the manual has been updated accordingly.

Fixes #1671.

Change-Id: lc1d853a4fb6c70c81c3969d3d8ba86f52956ef67

History

#1 - 01/14/2015 05:50 PM - Mark Abraham
Fair enough. For the record, these are only used by analysis tools.

#2 - 01/14/2015 05:58 PM - Chris Neale
Not entirely true. BOLTZ (used in repl_ex.c as part of the exchange acceptance criterion) derives from RGAS, which itself comes from BOLTZMANN and AVOGADRO.

#3 - 01/16/2015 05:59 PM - Mark Abraham
Right, good point

#4 - 06/18/2015 06:46 PM - Gerrit Code Review Bot
Gerrit received a related patchset `1` for Issue #1671.
Uploader: Erik Lindahl (erik.lindahl@gmail.com)
Change-Id: I9e52b2c2cbf592dad465189797f736c01b1924
Gerrit URL: https://gerrit.gromacs.org/4798

#5 - 06/18/2015 06:46 PM - Erik Lindahl
- Status changed from New to Fix uploaded

#6 - 06/18/2015 06:49 PM - Gerrit Code Review Bot
Gerrit received a related patchset `1` for Issue #1671.
Uploader: Erik Lindahl (erik.lindahl@gmail.com)
Change-Id: ld80c676fc12199bb682d6d62b3e7b8af0b5e808
Gerrit URL: https://gerrit.gromacs.org/4799
Gerrit received a related patchset '1' for Issue #1671.
Uploader: Erik Lindahl (erik.lindahl@gmail.com)
Change-Id: Ic1d853a4fb6c70c81c3969d3d8ba86f52956ef67
Gerrit URL: https://gerrit.gromacs.org/4743

- Status changed from Fix uploaded to Resolved

- Status changed from Resolved to Closed