Inclusion of possible options to an Entry

With reference to Memo CP-C/388, "Must compilers always use all possible options", several additional rules have recently been introduced concerning compilation options, among which are those mentioned in the Memo.

In this regard, it is suggested that while any possible option can be used in an Entry, the compiler only needs to include it in the Entry if he/she thinks it is important for the description of this particular experiment.

Memo CP-C/388

Date: 11 February 2010

To: Distribution

From: O. Schwerer

Subject: **Must compilers always use all possible options?**

I am increasingly confused by requests from NRDC colleagues (in their feedback on compilations) to use compilation options which are optional, in cases where these options are, in my opinion, not only not obligatory, but making things unnecessarily complicated both for the compiler and the user.

I therefore suggest to discuss this at the forthcoming NRDC meeting with the aim of either making (some of) these options obligatory (which in general I do not support), or to leave the decision to the compiler, as it was originally intended.

Two recent examples:

1) Requests to add the heading (MONIT)
to keywords MONITOR and MONIT-REF when only one monitor was used.

I believe that it is obvious for the user that the values of a single monitor reaction, defined under the keyword MONITOR, will appear in the DATA section under the heading MONIT.

Repeating the heading MONIT in the BIB section appears to me more confusing than helpful for the user and an unnecessary additional step for the compiler.

The option to code headings such as MONIT1, MONIT2 etc. under MONITOR, MONIT-REF and DECAY-MON is used when more than one monitor reaction needs to be coded, and should, in my opinion, normally be restricted to these cases.

2) Coding of natural isotopic abundances in coded form under SAMPLE

This option was introduced after a proposal in February 2009 (memo CP-D/546 of which I was a co-author). The possibility to code abundances of isotopes within a sample of natural isotopic composition was not meant to be a new obligation to compilers but an option to give these numbers when necessary, e.g. in cases of isotopes of very low abundance which are not as accurately known as the main isotopes, or when authors used an old value which is no longer up to date, or whenever the compiler considers it useful. However, in case of isotopes whose

abundance has been known accurately for a long time, for which authors give the values e.g. of NuDat, there should be no obligation to code them under SAMPLE.

While there can be cases where the use of a non-obligatory "option" can be recommended for a good reason, I am against automatic requests to always use all thinkable additional options, and I do not consider this to be always the best compilation practice.

I would welcome clarification of the two cases outlined above and, more generally, a confirmation that optional compilation possibilities are really optional rather than obligatory.

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