Subject: correct input of charged reference structures, evolutionary libraries
Posted by nbehrnd on Tue, 22 Aug 2023 16:53:31 GMT
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Dear Thomas,

while generating evolutionary libraries, DW can exclude/remove molecules with an unwanted structure feature. In an other thread,[1] you thankfully shared a .dwar file including a set of reference. It however equally includes entries with uncompensated charges or/and valences higher «than usual». An example is Me4N+ highlights by the question mark. (The attached .zip archive includes .dwar and screen photos as .png.)

By default, DW does not accept this entry in this form. Reading the .dwar in a separate session of DW, I edited the entry: removed the plus sign in DW's sketcher by a single click on the minus sign; with lasso Ctrl and left mouse click opened the window to select «Charge:» at level «has positive charge».

The structure of the ammonium appears to be fine in the visualization of the array, it is not in the display of the library generator: the charge seems absent, and (speculation:) because of the tetravalent nitrogen, the entry is not accepted as valid.

Subsequently, I assumed «any atom» with an assigned «has negative charge» could ease DW's action. However, while the generator view should be fine for for the absence of an overall charge, the carbanion now looks more like derived from methane, than «whatever anion». And displays again the question mark of an unfit entry. Dropping an alkyl substitution to Me3N+X- looked fine in the structure array, but again not fine as a reference structure: a neutral two component entry which however lost one alkyl chain .and. charges.

While it is possible to edit the entry from the sketcher invoked from the generator widget, it only was possible to generate Me4N+ and a CH_3^- anion; the liberty of defining any anion to compensate for the positive charge via lasso, Ctrl + left mouse boutton click seems currently absent.

My questions are:

+ how to enter such and similar charged motifs which are not a monoatomic ion as (earth) alkali cations or the halogenids
+ is entering them alone or altogether with a charge compensating entity already implemented / a possible extension of DW's functionality? This draws inspiration from amines seen reported as hydrochlorides, for example.
+ with similar tune as an earlier post: is adjusting the weight of this fitness criterion to 4.0 equivalent to render the restraint a constraint?

Best regards,

Norwid

[1] «Filter out nasty functions», https://openmolecules.org/forum/index.php?t=msg&th=662&start=0&, on <2023-07-14 Wed>

File Attachments

1) 2023-08-22_dw_valence_question.zip, downloaded 451 times