Subject: feature suggestion: .sdf export with explicit hydrogens
Posted by nbehrnd on Tue, 07 Sep 2021 08:10:50 GMT
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Dear Thomas,

for the already present export of structures generated by DW as an .sdf file (File -> Save Special -> SD-File), I would like to suggest an extension; namely that these files contain explicit hydrogens.

In the sketcher, the definition of e.g., fluorochlorobromomethane CHBrClF yields either (R), or (S) isomer. The .sdf generated however accounts for four atoms only where five (then including hydrogen) may be anticipated. Irrespective if the structures are flat 2D objects (e.g., result of generating a set of random molecules), a complete set of atom connectivities were helpful for processing the .sdf outside DW in other programs. While Chemistry -> Generate Conformers triggers the generation of a separate .dwar file from which the .sdf exported accounts for the hydrogen previously missing, I would welcome hydrogens included in the .sdf independently of this query.

Norwid