Subject: Re: search for conformers, empty column «minimization error»
Posted by thomas on Wed, 06 Apr 2022 09:56:37 GMT

Dear Norwid,

the minimization error column is populated in case the forcefield minimizer creates an error. A typical error would be a not supported atom type, because MMFF94 is limited to the usual organic atoms. I also noticed that if such an error occurrs, the energy field is empty and since there is an active filter, rows with empty energy values are filtered out unless one disables the filter. I now changed that and disable the filter automatically, when the file is created and there are rows with minimization errors.

Best wishes,

Thomas