Subject: Re: Error on attempting to generate conformers
Posted by thomas on Sat, 27 Aug 2022 10:14:48 GMT
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Hi Paul,

many thanks for reporting this serious issue. I was not aware of it, because I always tested with the capka.jar file in my classpath, which provides chemaxon pKa calculation. I had slightly changed the way, how that file would be recognized and used, which caused the problem. I have fixed and tested now with and without capka.jar.

Now conformer and property calculation work again in the newest dev version...

Thomas