Subject: Re: Copy and Paste 3D Pose Posted by thomas on Wed, 25 Jan 2023 11:50:40 GMT

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Hi Scott,

No, because when DataWarrior reads an SD-file, it creates a memory efficient molecule from that. The original SD-File content is not kept with a DataWarrior document. When reading from a 3D SD-file record, the relative orientation of the atoms is retained with a reasonable accuracy. The absolute position of the molecule is retained as well, but not exactly. Thus, when a new 3D-SD-file is created from the molecule, it will be moved slightly in space, which is typically much less than an Angstrom.

Thomas