
Subject: 3-D printing of chemical structures
Posted by [eperlste](#) on Thu, 27 Sep 2012 03:28:55 GMT
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Hello, I'm interested in producing 3-D molecules of methamphetamine.

Is the following link relevant: http://www.123rf.com/photo_8884006_3d-illustration-of-the-drug-methamphetamine-isolated-on-white.html

Thanks,
Ethan

Subject: Re: 3-D printing of chemical structures
Posted by [mkroeker](#) on Thu, 27 Sep 2012 07:02:46 GMT
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A "pay-per-use" stock picture of the desired structure is only semi-relevant to your question. Head over to Bristol university's molecule of the month collection at www.chm.bris.ac.uk/motm/motm.htm, find the Methamphetamine entry in the table and select its "vrmf" version (the "V" behind the name). Among the text, you will find a few illustrations of the molecule - click on them to download the 3d version. This file format should be printable on shapeways, even in color.

Subject: Re: 3-D printing of chemical structures
Posted by [eperlste](#) on Sat, 29 Sep 2012 04:32:02 GMT
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Thanks for the response! I'm still not clear what file extensions are compatible with 3D printing of chemical structures. I would like to produce a ball and stick model, like this: http://upload.wikimedia.org/wikipedia/commons/9/90/Methamphe_tamine2.png (with the N atom in blue, H in white, and C in dark gray).

Subject: Re: 3-D printing of chemical structures
Posted by [mkroeker](#) on Sat, 29 Sep 2012 12:31:01 GMT

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Did you check the link in my message ? While the chemical formula on that page is a conventional line drawing, the VRML (extension .wrl) file it links to is the color-coded 3D ball-and-stick model you want, and should be directly uploadable to shapeways.

Subject: Re: 3-D printing of chemical structures
Posted by [eperlste](#) on Sat, 29 Sep 2012 14:44:20 GMT
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I did! But it still wasn't clear to me that displayed image would be different than the .wrl file. Sorry, I'm a little slow, I guess!

Thanks for clarifying!

Subject: Re: 3-D printing of chemical structures
Posted by [eperlste](#) on Wed, 03 Oct 2012 13:17:45 GMT
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So I downloaded the .wrl version of the meth molecules from the link you suggested. The resulting files were 52kb in size. When I tried to upload them to Shapeways, I got an error.

Assume that in these matters you're dealing with a small child. Can I draw a structure in ChemDraw, export it, open it in Meshlab, and create a 3D compatible file?

Subject: Re: 3-D printing of chemical structures
Posted by [JACANT](#) on Wed, 03 Oct 2012 16:42:59 GMT
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It worked for me.

<http://www.shapeways.com/model/723440/methamphetamine.html>

http://www.shapeways.com/tutorials/exporting_to_vrml_and_x3d_for_color_printing

What size did you want?

Subject: Re: 3-D printing of chemical structures
Posted by [mkroeker](#) on Wed, 03 Oct 2012 17:14:54 GMT
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I see that JACANT beat me to it, thanks.
Regarding ChemDraw - probably yes, if it can export true 3D coordinates in the PDB format originally created for the Protein Data Bank ("true" 3D coordinates in the sense that they contain more than just the flat drawing with z=0 - I do not know ChemDraw's capabilities). The import options of meshlab for pdb appear to be quite limited, apparently it will create a "space-filling" model, but not a ball-and-stick one. The freeware RasMol program, however, should allow you to generate the kind of VRML file you want from a PDB one. Another alternative might be to try to find data from a crystal structure determination, e.g. in the "Crystallography Open Database" and work from there.

Subject: Re: 3-D printing of chemical structures
Posted by [7777773](#) on Wed, 03 Oct 2012 21:33:52 GMT
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You could also try Avogadro to model any chemical structure in 3D -
<http://avogadro.openmolecules.net>

Subject: Re: 3-D printing of chemical structures
Posted by [eperlste](#) on Sat, 06 Oct 2012 21:31:22 GMT
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Hello again. It's the idiot who's never used MeshLab or done any 3D printing. The good Samaritans on this forum directed me to the correct file:
<http://www.shapeways.com/model/723440/methamphetamine.html>

Now I would like to make the object 50% smaller. What's the easiest way to do that in MeshLab?
Thank you!

Subject: Re: 3-D printing of chemical structures
Posted by [mkroeker](#) on Sun, 07 Oct 2012 11:59:49 GMT

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Filters -> Normals, Curvatures and Orientation -> Transform:Scale
Set "XAxis" to 0.5, make sure that "Uniform Scaling" is checked, check the "Preview" box if you like, then click on "Apply" if you are satisfied with the settings.

Subject: Re: 3-D printing of chemical structures
Posted by [mkroeker](#) on Sun, 07 Oct 2012 13:20:22 GMT
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Oh well... VRML export from meshlab appears to be broken. And that wrl file is overly complex anyway - one extremely detailed mesh that just represents a tiny blue sphere that once must have been the anchor point for switching between the several viewer positions in the file. (And the molecule itself is a single mesh, not a collection of vrml "sphere" and "cylinder" primitives that would facilitate changing individual radii...)
Try this one here instead <http://shpws.me/k9gC> - i have removed the unnecessary viewpoints and the selector sphere, and added a scaling transformation at the top. Just open it in a text editor, find the line that reads "scale 0.5 0.5 0.5" and change it if necessary. (With this scale, an upload specifying "Inch" as the base unit results in a model that is 5 by 2.1 by 1.8 in and would cost something like \$15 in "full-color sandstone" or \$20 in paint-it-yourself WSF plastic.)

Subject: Re: 3-D printing of chemical structures
Posted by [JACANT](#) on Sun, 07 Oct 2012 18:22:58 GMT
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Please see updated file, half size. <http://www.shapeways.com/model/728611/>
As mkroeker pointed out there is a small isolated sphere approx .7mm. You can just see it in the center of the image. I don't think this will affect the print. Surely it will just get lost in the printing process. You could ask service@shapeways.com
