Poster Presentation

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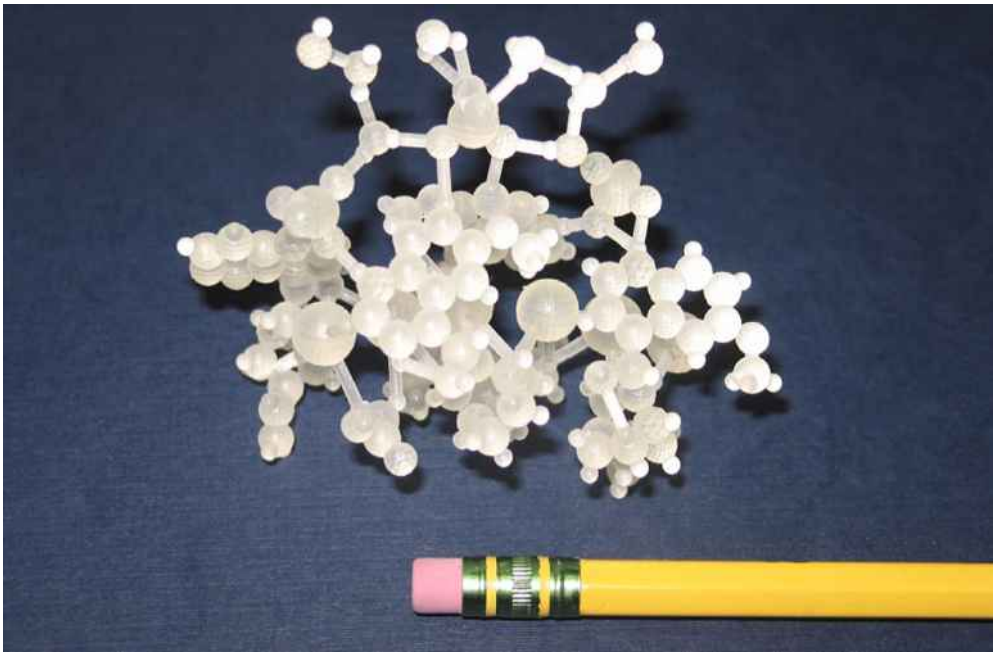
3D printing of crystallographic models and open access databases

W. Kaminsky[1], T. Snyder[2, 3], P. Moeck[3]

[1]University of Washington, Department of Chemistry, Seattle, Washington, USA, [2]XEROX, Wilsonville, Oregon, USA, [3]Portland State University, Department of Physics, Portland, Oregon, USA

Although introduced 30 years ago, cost and performance improvements have only recently made 3D printing affordable. The industry wide input file format for 3D printers incorporates explicit mesh - 'STL' data. Molecules and crystal structures, when including symmetry, crystal morphologies, or crystal defects are encoded in the parametrical 'CIF' syntax. Free software for converting directly CIF data to STL files has just been developed, available online [1]. First examples of printed 3D models from STL-files created with these programs include molecules of sucrose, herapathite [2a], caffeine, humulone [2b], an alpha-quartz crystal and its Japanese {112} twin or a brilliant cut diamond. Far more CIF encoded models are available, even open access. The Crystallography Open Database (COD) features over 245,000 entries and has recently developed into the world's premier open-access source for structures of small to medium unit cell-sized inorganic and molecular crystals [3a], complementing the well-established open-access Worldwide Protein Data Bank [3b]. The Cambridge Crystallographic Data Centre in the United Kingdom provides crystal structure data of small (organic) molecules free for bona fide research [3c]. Structural data on inorganic crystals, metals and alloys can be obtained free of charge from the Inorganic Material Database (AtomWork) [3d]. Related to the COD, the crystallographic open-access databases [3e] ("COD offspring") provide CIF data for interdisciplinary college education. With this basic infrastructure in place, any interested college educator may print out her or his favorite crystallographic structure model in 3D and use it in hands on class room demonstrations [3f].

[1] *[a] http://cad4.cpac.washington.edu/cif2vrmlhome/cif2vrml.htm, [b] http://cad4.cpac.washington.edu/WinXMorphHome/WinXMorph.htm,* ***[2]*** *[a] B. Kahr, J. Freudenthal, S. Phillips, W. Kaminsky, SCIENCE 324 (2009) 1407, [b] J. Urban, C. Dahlberg, B. Carroll, W. Kaminsky, Angew. Chem. 52 (2013) 1553-1555.,* ***[3]*** *[a] http://www.crystallography.net/, [b] http://www.wwpdb.org/ [c] http://www.ccdc.cam.ac.uk/Community/Requestastructure/Pages/DataRequest.aspx?. [d] http://crystdb.nims.go.jp/index_en.html. [e] http://nanocrystallography.research.pdx.edu. [f] Support fro*



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