MOLECULAR MODELING AND CREATING 3D MODELS OF CHEMICAL COMPOUNDS IN BLENDER SOFTWARE USING THE RESOURCES OF CHEMSPIDER AND OPEN BABEL

Phd Tihomir Dovramadjiev
Mechanical Engineering Faculty, Industrial Design Department - Technical University of Varna, Bulgaria.
tihomir.dovramadjiev@gmail.com

Abstract: *Creating 3D models of molecules and chemical compounds is a necessity in scientific work, which examines different states, structures, processes and interaction of molecules. This is done through the use of comprehensive 3D graphics programs as well as specialized applications containing and maintaining a database of ready-made models. The ability to work with good 3D graphics platform such as Blender combined with available resources of ChemSpider and Open Babel, builds a powerful system allowing the creation of high-quality and realistic virtual models of molecules and chemical compounds.*

Keywords*: Chemical, molecules, compounds, ChemSpider, Open Babel, Blender*

1. Problem discussion

The use of modern technological tools for designing molecules and compounds is an advantage that ensures reliability and speed in the workflow. Very good compatibility to the final modeling in Blender's software [1 - 10] have the utilities ChemSpider [11 - 13] providing molecular resources and Open Babel, as a tool for converting the required file formats [14 - 16]. This study aims to explore possibilities for providing the necessary virtual 3D molecules and chemical compounds used in modern practice and science.

2. Objective and research methodologies

For the purposes of the study a 3D virtual model of Hydroxyapatite (chemical formula $HCa_5O_{13}P_3$) will be provided. This important model is used for creation of computer simulations and animations in Blender environment with support of ChemSpider and Open Babel.

ChemSpider is a freely available database based on chemical structures, that provides information on over 26 million de-duplicated compounds derived from over 400 sources. These sources include a wide variety of government databases, chemical supplier catalogs, academic and commercial websites. Each of the listed sources has a brief popup description, with the full record providing a web link to the source. ChemSpider augments the default information from these sources with additional of property data (official website: http://www.chemspider.com). Possibilities of the ChemSpider free chemical database are shown on Fig. 1.

Fig. 1. ChemSpider - the free chemical database. ChemSpider search engine results: Systematic Name, Synonym, Trade Name, Registry Number, SMILES, InChI or CSID

In a real environment $HCa_5O_{13}P_3$ occupies an important place in medicine and implantology in particular, where is applied as a coating and has bioactive function [17 - 19]. Fig. 2 shows 2D view of $HCa_5O_{13}P_3$ and it's parameters. Fig. 3 shows 3D image (JSmol) of $HCa_5O_{13}P_3$.

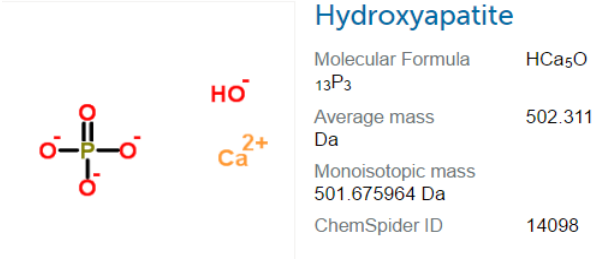


Fig. 2. 2D view of Hydroxyapatite. Molecular Formula $HCa_5O_{13}P_3$. Average mass 502.311 Da Monoisotopic mass 501.675964 Da ChemSpider ID 14098

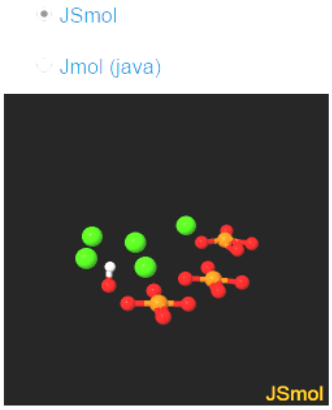


Fig. 3. 3D (JSmol) View of Hydroxyapatite ($HCa_5O_{13}P_3$). (http://www.chemspider.com/Chemical-Structure.14098.html?rid=376769cf-b675-44b6-b4ed-c475ae68ccce).

The file from the basis of ChemSpider is downloaded in * .mol format with number 14 098 (as listed in the database). To prepare $HCa_5O_{13}P_3$ model for work first it must be synchronized with the Open Babel (fig. 4) (source Open Babel: An open chemical toolbox).

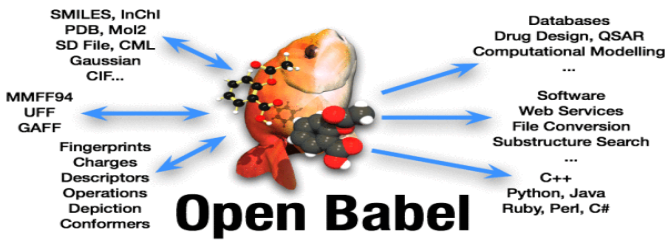


Fig. 4. Open Babel - open source chemical toolbox [14]

Open Babel is a chemical toolbox designed platform which can: search, convert, analyze, or store data from molecular modeling, chemistry, solid-state materials, biochemistry, or related areas. Open Babel is a project to facilitate the interconversion of chemical data from one format to another – including file formats of various types. This is important for the following reasons: multiple programs are often required in realistic workflows; many programs have individual data formats, and/or support only a small subset of other file types; chemical representations often vary considerably (some programs are 2D; some are 3D; some use fractional k-space coordinates; some programs use bonds and atoms of discrete types.; others use only atoms and electrons; some programs use symmetric representations - others do not; some programs specify all atoms - others use “residues” or omit hydrogen atoms). Open Babel Documentation Release 2.3.1. Providing (download) a fully functional open source program Open Babel can be done on the official website http://openbabel.org/, following the footsteps. Synchronization of 3D model $HCa_5O_{13}P_3$ obtained from Chem Spider in Open Babel is provided as it is defined in the field "Input format", using format: "mol-- MDL MOL format". The working file is opening with the following data for the model shown in Fig. 4. Processing of $HCa_5O_{13}P_3$ virtual model in PDB is possible by building a 3D coordinate system and determine the location of molecules. In the "Output format", is determined using format: "pdb - Protein Data Bank format". In panel settings are enabled: "Add hydrogens" and "Generate 3D coordinates". Following the conversion data a result is obtained with values shown in Fig. 5.

```
21 12  0  0000  0  0  0  0  0999 V2000
   6.1418   -2.2585    0.0000 Ca  0  2  0  0  0  0  0  0  0  0  0  0
   6.1418   -2.2585    0.0000 Ca  0  2  0  0  0  0  0  0  0  0  0  0
   6.1418   -2.2585    0.0000 Ca  0  2  0  0  0  0  0  0  0  0  0  0
   6.1418   -2.2585    0.0000 Ca  0  2  0  0  0  0  0  0  0  0  0  0
   6.1418   -2.2585    0.0000 Ca  0  2  0  0  0  0  0  0  0  0  0  0
   1.2861   -1.9950    0.0000 P   0  0  0  0  0  0  0  0  0  0  0  0
   1.2861   -1.9950    0.0000 P   0  0  0  0  0  0  0  0  0  0  0  0
   1.2861   -1.9950    0.0000 P   0  0  0  0  0  0  0  0  0  0  0  0
   1.2861   -3.3250    0.0000 O   0  5  0  0  0  0  0  0  0  0  0  0
   2.6600   -1.9950    0.0000 O   0  5  0  0  0  0  0  0  0  0  0  0
   0.0000   -1.9950    0.0000 O   0  5  0  0  0  0  0  0  0  0  0  0
   1.2861   -3.3250    0.0000 O   0  5  0  0  0  0  0  0  0  0  0  0
   2.6600   -1.9950    0.0000 O   0  5  0  0  0  0  0  0  0  0  0  0
   0.0000   -1.9950    0.0000 O   0  5  0  0  0  0  0  0  0  0  0  0
   1.2861   -3.3250    0.0000 O   0  5  0  0  0  0  0  0  0  0  0  0
   2.6600   -1.9950    0.0000 O   0  5  0  0  0  0  0  0  0  0  0  0
   0.0000   -1.9950    0.0000 O   0  5  0  0  0  0  0  0  0  0  0  0
   1.2861   -0.6650    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
   1.2861   -0.6650    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
   1.2861   -0.6650    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
   6.2736    0.0000    0.0000 O   0  5  0  0  0  0  0  0  0  0  0  0
  6  9  1  0
  6 10  1  0
  6 11  1  0
  6 18  2  0
  7 12  1  0
  7 13  1  0
  7 14  1  0
  7 19  2  0
  8 15  1  0
  8 16  1  0
```

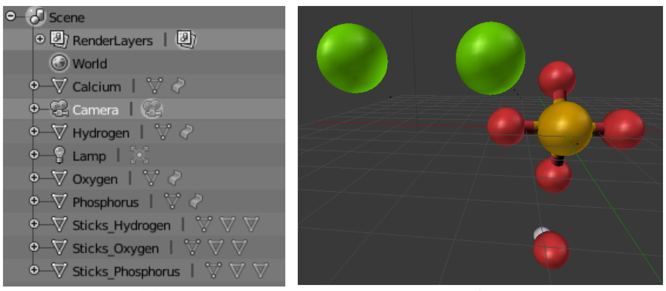
(a)

```
COMPND    UNNAMED
AUTHOR    GENERATED BY OPEN BABEL 2.3.2
HETATM  1 CA  LIG   1     1.056  -0.062  -0.055  1.00  0.00       Ca2+
HETATM  2 CA  LIG   2     1.056  -0.062  -0.055  1.00  0.00       Ca2+
HETATM  3 CA  LIG   3     1.056  -0.062  -0.055  1.00  0.00       Ca2+
HETATM  4 CA  LIG   4     1.056  -0.062  -0.055  1.00  0.00       Ca2+
HETATM  5 CA  LIG   5     1.056  -0.062  -0.055  1.00  0.00       Ca2+
HETATM  6 P   LIG   6     1.056  -0.062  -0.055  1.00  0.00       P
HETATM  7 P   LIG   7     1.056  -0.062  -0.055  1.00  0.00       P
HETATM  8 P   LIG   8     1.056  -0.062  -0.055  1.00  0.00       P
HETATM  9 O   LIG   6     1.056  -0.610  -1.695  1.00  0.00       O1-
HETATM 10 O   LIG   6     1.056  -1.209   1.241  1.00  0.00       O1-
HETATM 11 O   LIG   6    -0.674  -0.062  -0.055  1.00  0.00       O1-
HETATM 12 O   LIG   7     1.056  -0.610  -1.695  1.00  0.00       O1-
HETATM 13 O   LIG   7     1.056  -1.209   1.241  1.00  0.00       O1-
HETATM 14 O   LIG   7    -0.674  -0.062  -0.055  1.00  0.00       O1-
HETATM 15 O   LIG   8     1.056  -0.610  -1.695  1.00  0.00       O1-
HETATM 16 O   LIG   8     1.056  -1.209   1.241  1.00  0.00       O1-
HETATM 17 O   LIG   8    -0.674  -0.062  -0.055  1.00  0.00       O1-
HETATM 18 O   LIG   6     2.601  -0.062  -0.055  1.00  0.00       O
HETATM 19 O   LIG   7     2.601  -0.062  -0.055  1.00  0.00       O
HETATM 20 O   LIG   8     2.601  -0.062  -0.055  1.00  0.00       O
HETATM 21 O   HOH   9     1.056  -0.062  -0.055  1.00  0.00       O1-
HETATM 22 H   HOH   0     2.026  -0.062  -0.055  1.00  0.00       H
CONECT  6  9 10 11 18
CONECT  6
CONECT  7 12 13 14 19
CONECT  7
CONECT  8 15 16 17 20
CONECT  8
CONECT  9  6
CONECT 10  6
```

(b)

Fig. 5. Open Bible data conversation (a) Input format: mol-- MDL MOL format of $HCa_5O_{13}P_3$ (b) . Output format: pdb -- Protein Data Bank format of $HCa_5O_{13}P_3$.

The resulting data is saved in a file with the extension * .PDB. (HA.PDB). The file is imported into Blender software, through activation of Atomic Blender - PDB Addon (File → User Preferences → Import-Export Atomic Blender - PDB. The file containing the data for $HCa_5O_{13}P_3$ is used for simulations, animations and visualizations for assignment. Fig.6(a) shows the configuration of the defined $HCa_5O_{13}P_3$ and Fig.6(b) shows visualization of 3D models in Blender's environment.



(a) (b)

Fig. 6. 3D model of $HCa_5O_{13}P_3$ in Blender's environment (a) configuration (b) visualization

Using the same methodology other molecules and compounds can be used, to be added to the existing ones, to be modified and examined.

3. Conclusion

Finding and using available open source reservoirs which have data for the needs of modern science, and especially biology, medicine, biomedicine, chemistry and others is particularly relevant at the moment. This is possible due to the rapidly increasing volume of information, delivery to accessible repositories of information and easy access. A very good example is ChemSpider, where incoming information data is scientifically confirmed. On the other side the data is easily converted to Open Babel and becomes fit for further research in Blender software, which allows to carry out many successful actions and developments on assignment.

References

[1]. Tihomir Dovramadjiev. Modern accessible application of the system blender in 3d design practice. International scientific on-line journal "SCIENCE & TECHNOLOGIES" Publisher "Union of Scientists - Stara Zagora". ISSN 1314-4111 140. Bulgaria, 2015. 10 - 13p.

[2]. Felician Alecu, Blender Institute – the Institute for Open 3D Projects, Open Source Science Journal Vol. 2, No. 1, Economic Informatics Department, ASE Bucharest, Romania, 2010, 36 – 45p.

[3]. Ami Chopine, 3D Art Essentials The Fundamentals of 3D Modeling, Texturing, and Animation, Elsevier, ISBN: 978-0-240-81471-1, USA, 2011, 249 – 252p.

[4]. John M. Blain. Computer Modeling and Animation. The Complete Guide to Blender Graphics. Taylor & Francis Group, LLC. ISBN:13: 978-1-4665-1704-2. UK, 2012.

[5]. А.А.Прахов, Blender: 3D-моделирование и анимация. СПб.: БХ В, ISBN 978-5-9775-0393-8, Русия, 2009, 272 с: ил.

[6]. Ami Chopine, 3D Art Essentials The Fundamentals of 3D Modeling, Texturing, and Animation, Elsevier, ISBN: 978-0-240-81471-1, USA, 2011, 249 – 252.

[7]. Felician Alecu, Blender Institute – the Institute for Open 3D Projects, Open Source Science Journal Vol. 2, No. 1, Economic Informatics Department, ASE Bucharest, Romania, 2010, 36 – 45.

[8]. James Chronister, Blender 3D Basics 3rd Edition, Creative commons attribution NonCommercial-share alike 3.0 Unported License, 2009,146 p.

[9]. Lance Flavell, Beginning Blender - Open Source 3D Modeling, Animation, and Game Design, Apress, ISBN-13 (pbk): 978-1-4302-3126-4, USA, 2010.

[10]. Roger D. Wickes, Foundation Blender Compositing, ISBN-13 (pbk): 978-1-4302-1976-7,USA, 2009.

[11]. Pence, H. E. & Williams, A. (2010). ChemSpider: An Online Chemical Information Resource, Journal of Chemical Education 87 : 1123-1124.

[12]. Crystallography Open Database (COD). Vilnius University Press. 2014. 12-13p.

[13]. M. Rabie and C. M. Franck. Predicting the electric strength of proposed sf6 replacement gases by means of density functional theory. 18th Int. Simp. of high voltage engineering. South Korea, 2013. 1381 - 1386p.

[14]. Noel M. O’Boyle. Open Babel. Access and interconvert chemical information. Open Babel development team and NextMove Software. Cambridge, UK, 2013. 39p.

[15]. Enade Perdana Istyastono. Construction and optimization of structure-based virtual screening protocols to identify cyclooxygenase-1 inhibitors using Open Babel, spores and plants. Indo. J. Chem., Indonesia 2012, 12 (2), 141 - 145p.

[16]. Geoffrey R Hutchison Chris Morley Craig James Chris Swain Hans De Winter Tim Vandermeersch Noel M O’Boyle (Ed.). Open Babel Documentation. Release 2.3.1. 2012. 145p.

[17]. Abdulaziz Binahmed, Andrew Stoykewych, Ali Hussain, Brock Love, Vijay Pruthi. Long-Term Follow-up of Hydroxyapatite-Coated Dental Implants—A Clinical Trial. The International Journal of Oral & Maxillofacial Implants. Quintessence Publishing Co. 2007, 963 - 968 p.

[18]. A. Jemat, M. J. Ghazali, M. Razali and Y. Otsuka. Surface Modifications and Their Effects on Titanium Dental Implants. Hindawi Publishing. Egypt, 2015. 11p.

[19]. A Simunek, D Kopecka, M Cierny, I Krulichova. A Six-Year Study of Hydroxyapatite-Coated Root-Form Dental Implants. West Indian Med J 2005; 54 (6): 393 - 397p.