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Drawing, Modeling and Information

ChemOffice Reviews

Obtaining Beautiful 3D Drawings

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Dr. Michael K. Engel, a Guest Research Associate at the Kawamura Institute of Chemical Research, Japan, is currently working in the field of synthesis and application of metal-containing organic macrocycles. He is especially interested in investigating the influence of molecular and crystal structures on material properties.

He would like to see more 3-dimensional structural drawings in publications and recommends using ChemDraw and Chem3D, both part of the ChemOffice Ultra software package, as necessary tools for preparing such reports.

We Have Come A Long Way Since The Irksome Times of Drawing Figures

With the aid of templates, rulers and drawing ink, or the infurating task of retyping a whole

page of text purely because we had made an error in the final sentence. Fortunately, this is all history, and nowadays we have the use of sophisticated word-processing and chemical-drawing utilities at our fingertips, software about which we had previously not even dreamed. One such drawing package is ChemDraw, a tool which has accompanied me from my time as a graduate student through to the present. Indeed, with every new update, ChemDraw has continually surprised me with its range of new and improved functions.

One outcome of this readily available and easy-to-use desk-top publishing software is the 'you-have-to-use-it' policy, as stated by the various scientific publishers. If one plans to publish research in a renowned journal, then the drawings have to meet a certain criteria to conform with the settings specified by the journal's publisher. Thankfully, ChemDraw not only offers style-sheets which allow users to apply different settings (line-widths, etc.) to drawings, but also enables them to save drawings in a variety of formats. This feature is a necessity since most editorial offices require the structure files as well as the print-outs, generally in the form of TIFF (Tagged Image File Format) or EPS (Encapsulated Postscript) formats.

To Finally Obtain Beautiful 3-D Structural Drawings

Despite the many useful and helpful possibilities which are provided by modern chemical drawing software, there are still many drawings which are visually displeasing. Among them are, for example, some [60]fullerenes, which resemble semi-inflated soccer balls rather than the highly symmetrical spheres which they are supposed to represent. The problem with such drawings lies in the fact that the images formed are a result of our own direct translation of a two-dimensional drawing into a three-dimensional model. Consequently, the perceived 3-D image is often riddled with inaccuracy due to there being mistakes in the bond lengths, bond angles or projection geometry. However, with the aid of Chem3D and ChemDraw, both products contained in the various ChemOffice packages, it is easy to avoid unpleasant pictures and produce more attractive 3D images. To achieve this, one can either start with the molecules' 2-D drawing or with its crystallographic or calculated structural data.

With ChemOffice It's Very Easy

We shall use triptycene as an example to show how to start with a drawing.

1. Start ChemDraw and construct a triptycene molecule by connecting the 9 and 10 positions of 9,10 dihydroanthracene with the two ortho positions of a benzene ring (Figure 1a). Save the result as a ChemDraw file and close the window.

2. Reopen this file using Chem3D and perform an energy minimization. This results in the triptycene molecule together with its three-dimensional structure data. By choosing an appropriate view, one can obtain a drawing similar to that shown in Figure 1b).

3. Edit this figure to remove the double bonds, which are not necessary in cases where only the positions of the atoms are of interest. To remove the double-bonds while keeping the obtained structure one must deselect Correct Atom Types and Apply Standard Measurements in the Building control panel situated in the Preferences dialog. The drawing should now look like that shown in Figure 1c).
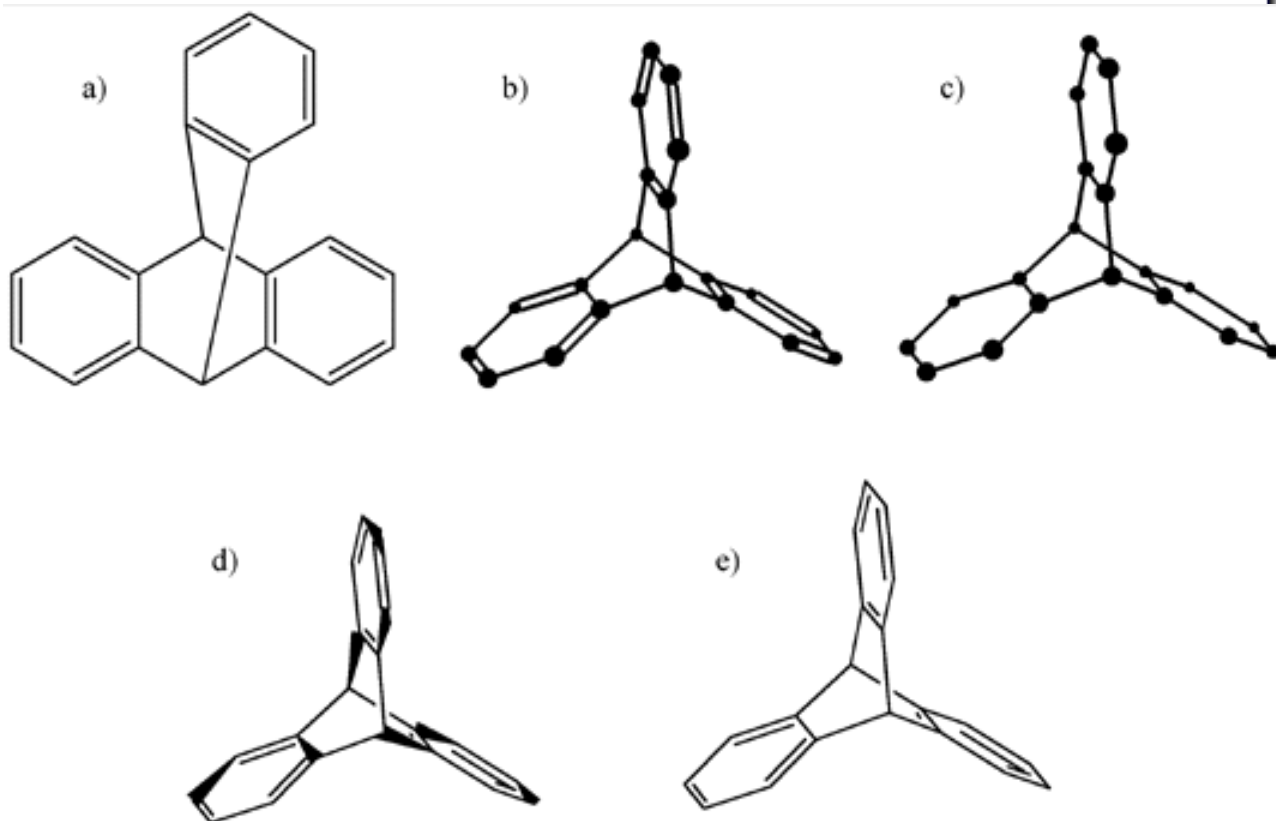
Figure 1. Triptycene molecular structures

4. This picture can now be transferred into other applications, e.g., a wordprocessor or back into ChemDraw using the clipboard function. However, with this method the picture cannot be edited in those applications which are linked to the original software by Object Linking and Embedding (Windows) or Publishing and Subscribing (Macintosh) protocol. If one needs to obtain a structure which can be altered in other documents without opening the original application, then a slightly different method is required (steps 5-7).

5. Follow steps 1 and 2 to obtain the structure shown in Figure 1b). Instead of exporting the structure from Chem3D via the clipboard function, choose the Save As command and export the structure as a ChemDraw file.

6. Reopen this file with ChemDraw to obtain the structure shown in Fig. 1d), where the spatial arrangement of bonds and atoms is illustrated by various Solid-Wedged Bonds. This structure can now be edited, for example, through exchanging atoms, or adding substituents.

7. By selecting the Solid Bond function in the left-hand Tools Palette and double-clicking the wedged bonds in the triptycene structure, one is able to exchange these wedged bonds for single-bonds (Figure 1e). I personally prefer this kind of drawing, because we are able to visualize the exact 3-D orientation of the structure, i.e. correctly determining which bond points out of the plane of the paper and which one points inwards.

8. There is still one better method for displaying 3-D structures - the use of stereoviews. However, the main drawback with these images is that they consume more space than normal figures and editors will only accept them if their use is justified. To obtain a stereoview, follow steps 1, 2 and 3 to form the structure shown in Figure 1c). Then select Display Stereo Views in the Stereoviews control panel of the preference menu to produce a "left-eye" and a "right-eye" image on the screen. By exporting this figure and pasting it into either a wordprocessor file or ChemDraw itself, one can obtain a print-out of the structure (Figure 2) and view it using a

stereoscope (stereoscopic glasses). It should be mentioned, however, that with some stereoscopes the figure obtained must be reduced by 50% before the left- and right-eye images can match, so producing the final 3-D image.
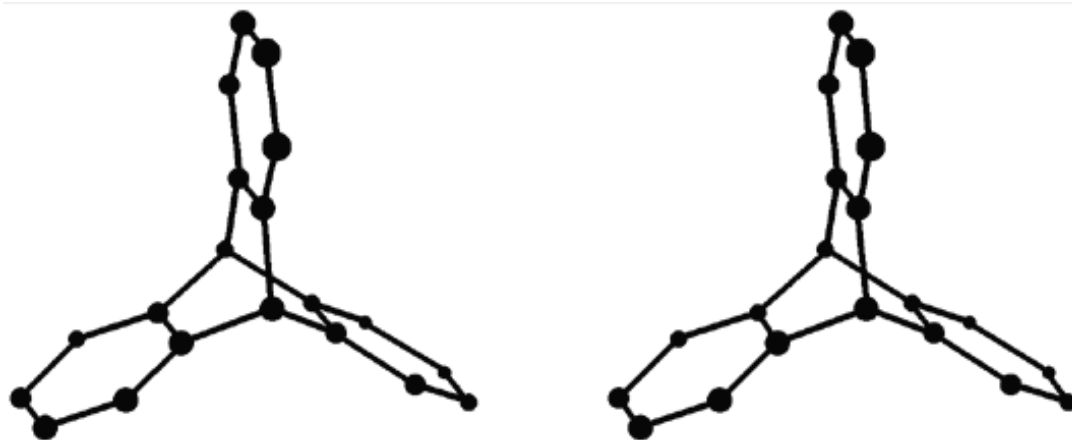

Figure 2. Stereoview of the triptycene molecular structure

And Very Quick

One can cut short the method for producing 3D drawings if the coordinates of a single-crystal structure or the structural calculation data are available. Chem3D can recognize and import structures from all important structure formats: Alchemy, Cartesian Coordinates, Cambridge Crystal Data Bank, Connection Table, Internal Coordinates, Macro Model, MDL Molfile, Mopac Input, Protein Data Bank (PDB), Standard Molecular Data or Sybyl. After importing such a structure, it can then be easily transformed into a 3-D image using one of the methods described above.

To explain the results of my structural research, I am often required to produce 3-D drawings from single-crystal data. To do this, I generate a PDB file on my Macintosh from the crystallographic display software, edit the structures using Chem3D and then save it to any file format which colleagues are able to read and edit using PC-based software. Additionally, I also create ChemDraw drawings for reports or publications, where even complicated structures, such as these taken from my review concerning single-crystal structures of phthalocyanines1, a group of very important organic pigments, are easy to understand (Figure 3).
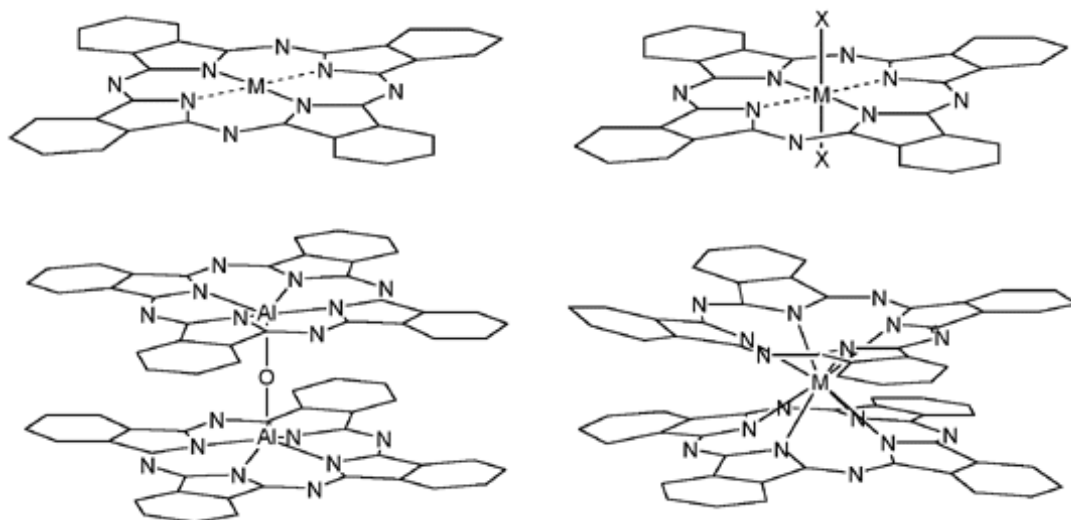

Figure 3. Molecular structures of some phthalocyanine complexes

Conclusion

Since I first met some weeks ago with the new ChemOffice Ultra, I enjoyed very much using it. Compared with ChemOffice Pro 3.5, which I have installed on my Mac powerbook, Chem Office Ultra is a vast improvement. I personally recommend it to beginners as well as to 'power users'. Both will find it very useful and ask themselves how they could have lived without. I would especially like to express my appreciation of the very informative and well-written handbooks which makes using ChemOffice Ultra so easy. Other software producers should take note at how handbooks can be written. Chem Office Ultra will show its extraordinary strength in a multi-system computer environment through the possibility to share easily files.

Rating: 5 flasks

1) Single Crystal and Solid-State Molecular Structures of Phthalocyanine Complexes
M. K. Engel, *Report Kawamura Inst. Chem. Res.*, 8 (Vol.Date 1996), 11-54 (1997); CA 127:313213.